Aspen simulation of biomass conversation processes

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Abstract

This study aims to develop a simulation model of the main operations in a pelletization process: combustion of biomass, solid separation, and drying of fresh biomass to be converted into pellets.

This simulation will allow the use of several types of biomass, with minimal effort from the user. The results were compared and adjusted according to the pellets industrial plant data. Different integration scenarios will also be analysed to convert the excess heat of the process into electricity and useful heat. A simple gasification model was developed to reproduce the results of an experimental study.

1. Introduction

Energy consumption has been steadily increasing in the last centuries, relying mostly on the use of fossil fuels. Resource management and environmental impact is forcing to a change of paradigm and consequent investment in renewable energy sources.

Biomass presents an attractive option due to the possibility of generating thermal energy, electricity and biofuels. Thermal energy can be produced through the direct conversion of biomass, while electricity can only be generated with an intermediate fluid (steam) in a Rankine cycle. Biofuels and valuable bio products may also be obtained by thermochemical or biochemical processes (Figure 1).

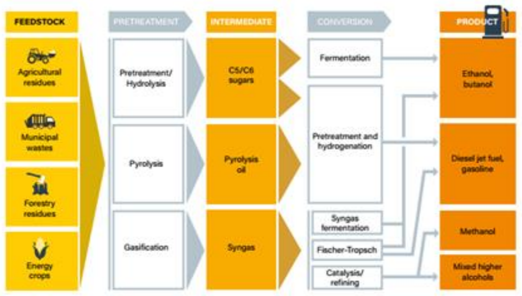


Figure 1 – Different technologies to produce biofuels (REN21, 2017)

The use of simulators, like Aspen Plus, is useful to reproduce the behaviour of the industrial processes aforementioned, and consequently allow offering valuable insight during study and optimization of these processes.

Combustion and drying models have been developed by Aspentech, but these ones require a permanent input of calculated parameters when considering different raw materials and operational conditions. The present work deals with the construction of an automatic model that simulates the process and enables consequent analysis of different operational conditions, biomass types and flowrates.

This work studies the main operation units of a pelletization process (combustion, solid separation and drying), as presented in Figure 2.

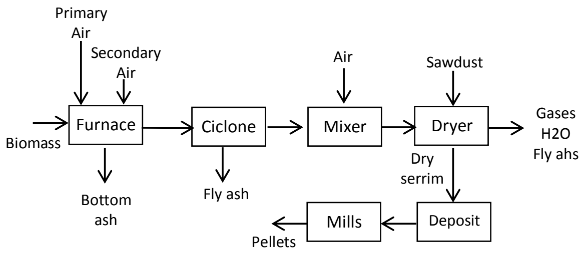
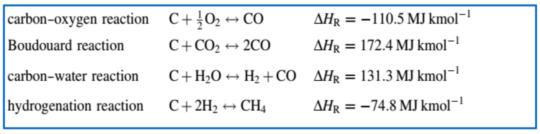


Figure 2 – Different technologies to produce biofuels (REN21, 2017)

This process generates high temperature streams. Thus, to increase the global efficiency of process it was analysed different integration scenarios which includes the production of electricity, circulating through a turbine the steam produced in the boiler. Cogeneration will also be analysed since the thermal energy generated simultaneously with electricity will be used in the process.

A gasification model was also explored through several steps: drying, fast pyrolysis and gasification. Drying consists in reducing the biomass moisture content to at least 20%. Fast pyrolysis is the production of biochar and bio oil through rapid and intense heating (approximately at 500°C) of the biomass feed. Gasification consists in gas-solid reactions (Figure 3) and gas-gas reaction between biochar and the reaction gas (steam, air or oxygen).



carbon–oxygen reaction	$C + \frac{1}{2}O_2 \leftrightarrow CO$	$\Delta H_R = -110.5\ \mathrm{MJ\ kmol^{-1}}$
Boudouard reaction	$C + CO_2 \leftrightarrow 2CO$	$\Delta H_R = 172.4\ \mathrm{MJ\ kmol^{-1}}$
carbon–water reaction	$C + H_2O \leftrightarrow H_2 + CO$	$\Delta H_R = 131.3\ \mathrm{MJ\ kmol^{-1}}$
hydrogenation reaction	$C + 2H_2 \leftrightarrow CH_4$	$\Delta H_R = -74.8\ \mathrm{MJ\ kmol^{-1}}$

Figure 3 – Gas-solid reactions

2. Biomass characterization

Different biomass may be characterized, in dry basis, by its proximate and ultimate analysis. These analyses include ash and chlorine content. However, Aspen Plus only accepts feeds if:

1. ash content of proximate and ultimate analysis are the same;
2. sulphur content of ultimate analysis is equal to sulphate content, of the sulphate analysis.

Vassilev et al. (2010) present a review of proximate and ultimate analysis for different biomass feeds. Table 1 and Table 2 summarize those analyses. The ultimate analysis was modified according to the requested Aspen format.

Table 1 – Proximate analysis, (Vassilev et al., 2010; Ferreira, 2015)

nº	Type	Volatile matter	Fixed carbon	Ash
1	Martos biomass	0	97,8	2,2
2	Eucalyptus bark	78	17,2	4,8
3	Forest residues	79,9	16,9	3,2
4	Pine bark	73,7	24,4	1,9
5	Pine sawdust	83,1	16,8	0,1
6	Agriculture residues	75,2	19,1	5,7
7	Corn straw	73,1	19,2	7,7
8	Rice straw	64,3	15,6	20,1
9	Wheat straw	73,4	15,8	10,8
10	Straw	74,8	18,1	7,1
11	Olive wood	79,6	17,2	3,2

Table 2 – Biomass ultimate analysis (Aspen format) (Vassilev et al.,2010; Ferreira, 2015)

nº	Type	Carbon	Oxygen	Hydrogen	Nitrogen	Sulphur	Chloride
1	Martos biomass	2,20	59,94	34,46	3,30	0,09	0,01
2	Eucalyptus bark	4,77	46,23	43,01	5,41	0,25	0,29
3	Forest residues	3,24	50,98	39,76	5,22	0,68	0,10
4	Pine bark	1,89	49,90	41,97	5,87	0,29	0,07
5	Pine sawdust	0,12	50,93	42,84	5,99	0,10	0,01
6	Agriculture residues	5,80	46,89	40,03	5,83	1,13	0,14
7	Corn straw	7,67	44,69	40,47	5,87	0,64	0,07
8	Rice straw	20,1	39,8	34,2	4,5	0,8	0,1
9	Wheat straw	7,12	45,62	40,26	5,63	0,65	0,16
10	Straw	10,85	43,26	39,45	4,96	0,89	0,12
11	Olive wood	3,21	47,41	43,45	5,23	0,68	0,03

3. Direct Combustion

The furnace is an equipment where occurs the combustion (ex: biomass) with air, giving rise to combustion gases at relatively high temperatures. Aspen Plus® simulator does not have its own model for furnace simulation. So, a furnace was defined, using a set of blocks outlined in Figure 4.

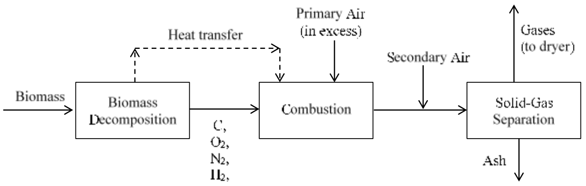


Figure 4 – Furnace block diagram

The furnace, where the combustion of biomass with air occurs, was simulated in Aspen Plus using different Aspen models, such as RYield and RGibbs reactors, Mixer, Split Separator and Heater (see Figure 5). A brief description of the different process blocks is given below:

Furnace 1 – RYield reactor: Inputs – reaction yield distributions (obtained in "Combust calculator" using proxanal, ultanal e sulfanal analysis).

Furnace 2 – RGibbs reactor: Inputs: heat of biomass decomposition (from Furnace 1); air flow rate that is obtained in "Air calculator" using the biomass flow rate and the percentage of excess of air.

Furnace 1 and Furnace 2 simulate the biomass combustion, which is described by the following reaction:

$$\text{Biomass} + O_2 \rightarrow CO + CO_2 + SO_2 + H_2O + NO_x \qquad (1)$$

Furnace 3 – "Mixer": the temperature of the combustion gases that are sent to the dryer is adjusted to the required value through the addition of air.

Furnace 4 – "Split": separation of ash from the gases of combustion.

Furnace 5 – Heater: the temperature of the combustion gases is recalculated using furnace efficiency (EFF calculator).

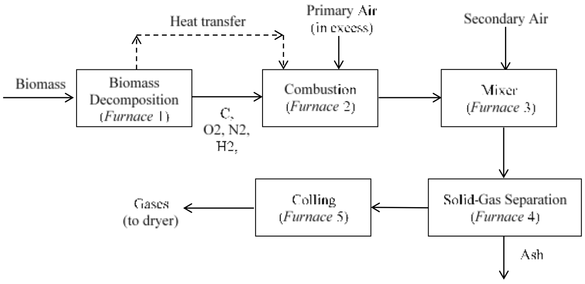


Figure 5 – Furnace block Aspen diagram

The results obtained in the Aspen simulation, using input data corresponding to the base case of an industrial pellets unit (Table 3), are presented in Table 4.

Table 3 – Industrial pellets plant data (input in Aspen furnace simulation)

Biomass type	Wood chips
Biomass to furnace	1760 kg/h
%H Furnace biomass	44%
%Ex air primary	40%
Sawdust to pellets	7000 kg/h
%H sawdust	40%
%H dry sawdust	10%
Furnace efficiency	95%

Table 4 – Aspen simulation results for the furnace block using input data from Table 3.

	Primary air (AIR)	*Secundary air (AIRSEC)*	*Furnace out (PRODUCTS)*	*Mixer in (PROD2)*
T (ºC)	15,5	15,5	1121.5	850
H_2O	75,86285	33,47699	1174,402	1140,925
N_2	7097,103	3131,831	10229,81	7097,983
O_2	2181,699	962,7467	1651,954	689,2072
NO_2			0,0224	0,0224405
O_2S			0,197	0,1969
H_2			0,00024	0,00024
CL_2				
HCL				
CO			0,00546938	0,00546938
CO_2			2164,641	2164,641
H_2S				
BIOMASSA				
FASH			10,84	10,84
BASH			10,84	
Total	9354,	4128,0	15231,88	11114,66

4. Solid-Gas separation

The solid fraction in the combustion gas stream must be strongly decreased to avoid fouling problems in downstream operations. Perry's (2008) suggests for particle removal treatment a cyclone, a filter and an electrostatic precipitator. A cyclone and a filter were simulated in Aspen Plus. The method used for cyclone´s calculations was the *Muschelknautz*, which only requires the introduction of the pressure drop to calculate the operation's efficiency. A *DESIGN-SPEC was* implemented which sets the efficiency at 75%, and manipulates the pressure drop. This efficiency will be increased later, if necessary to follow Portuguese legislation, regarding particle emissions.

A filter was simulated according to a gas rate of 10 m/s and a pressure loss of 0,05 bar, corresponding to the maximum acceptable values by the simulator. Green (2008) points that the maximum temperature in filers is around

90°C, for natural fiber filters and 260°C for synthetic fiber ones, which considerably lower when compared with the process conditions.

The electrostatic precipitator needed the introduction of more detailed parameters, such as gas mixture dielectric constant. However, Green (2008) suggests an electrostatic precipitator efficiency of 91%.

The cyclone was chosen because it is the best economic option (Figure 6).

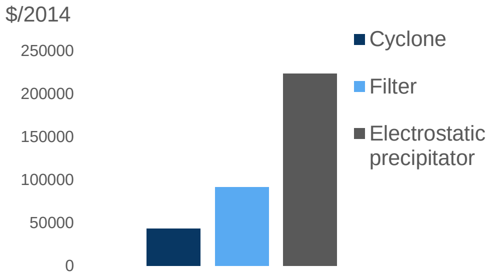


Figure 6 – Solid separation unit´s cost (Matche, 2017)

5. Drying operation

The production of pellets has an initial stage of sawdust drying. The flue gases will be used directly to perform this drying, being premixed with fresh air in a mixing chamber to achieve the temperature and the gas flow for the dryer's successful operation.

5.1. Analysis of the heat capacity for solids, calculated by Aspen Plus

Solid biomass is heated in the dryer in a large temperature range. Therefore, it was important to analyse how Aspen Plus deals with heat transfer in solids. Aspentech (2013) introduces different methods for heat capacity calculations, namely *Kirov* (Equation 2) and *Cubic Interpolation* (Equation 3).

$$Cp_{i,j} = a_{i,j1} + a_{i,j2}T + a_{i,j3}T^2 + a_{i,j4}T^3 \qquad (2)$$

where T (K), *i*, *j*, indexes of components and constituents(Aspentech, 2013(a));

$$Cp^d = a_{1i} + a_{2i}T + a_{3i}T^2 + a_{4i}T^3 \qquad (3)$$

where *T* (K) and *I the element index.*

Dupont (2010) propose a method to calculate the heat capacity of biomass solids described by Equation 3.

$$Cp_{biomassa} = 5{,}340T - 299\ (Jkg^{-1}K^{-1}) \qquad (4)$$

where *T* (K) and *I the element index.*

Because moisture content is quite high in biomass feeds, a study of the influence of this parameter on the heat capacity of the solid was carried out. Figure 7 compares the results of the heat capacity calculations as a function of the moisture content.

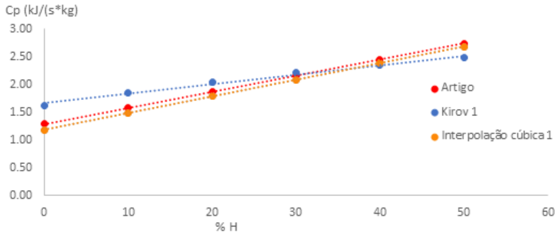


Figure 7 – Comparison of heat capacity methods (Dupont et al., 2013; Aspentech, 2013)

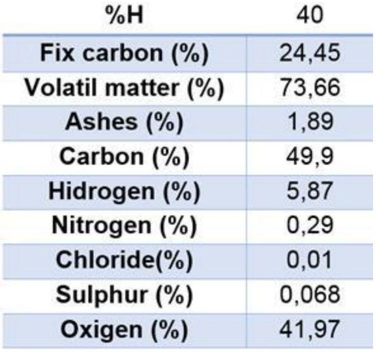
Figure 7 allows concluding that the Cubic Interpolation method presents the best approximation. This can be selected in the option Properties, of the simulator, in Methods>NCProps, third option of HCOALGEN, placing the index *2*.

5.2. Models of dryers

In the present work, several dryer options have been tested: the proposed solution by Aspentech (2013), the DRYER block presented in Aspen Plus, and a third alternative, using a MIXER block.

The main characteristics of sawdust, which will be dried to produce pellets, are presented in Table 5.

Table 5 – Input data for sawdust dryer



%H	40
Fix carbon (%)	24,45
Volatil matter (%)	73,66
Ashes (%)	1,89
Carbon (%)	49,9
Hidrogen (%)	5,87
Nitrogen (%)	0,29
Chloride(%)	0,01
Sulphur (%)	0,068
Oxigen (%)	41,97

5.2.1. Model of Dryer "Aspentech"

This model has been suggested to dry a coal stream. It consists of a block RSTOIC, controlled by a CALCULATOR, in which the drying occurs, and a FLASH2, where the gas-solid separation occurs, as shown in Figure 8.

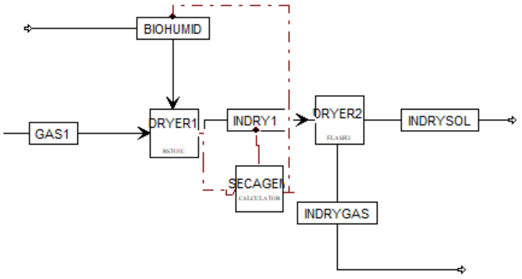


Figure 8 – Aspen blocks for dryer "Aspentech" model

Block RSTOIC, named DRYER1, introduces the drying reaction of non-conventional solids:

$$BIOMASSA\ (s) \rightarrow 0{,}0555084 H_2O\ (g) \qquad (5)$$

Aspen Plus assumes that biomass molecular weight is *1g/mol*, and therefore water must have a coefficient of *0,0555084 (1/18)*.

The CALCULATOR, SECAGEM, defines the moisture fraction in the dry sawdust and calculates the extent of the reaction in the RSTOIC (equation 6).

$$\frac{(H_2O_{entra} - H_2O_{sai})}{(100 - H_2O_{sai})} \qquad (6)$$

Block FLASH2, DRYER2, executes the separation, with a duty input of *0 Gcal/hr*.

5.2.2. Model of Dryer "DRYER BLOCK"

The "DRYER BLOCK" model makes use of the imbibed dryer block, presented in Aspen Plus. In order to work with this block one must access the Setup>Solids folder, and activate water as a moisture component. The heat duty must be 0 Gcal/hr, because the heat must come exclusively from the inlet streams. The simulation employed used WATER, in DRY basis, to a fraction of 0,1 in the output stream. This block requires detailed data, like drying curves that were not available.

5.2.3. Model of Dryer "MIXER BLOCK"

This model has no mass contact blocks during the drying phase, and only heat is exchanged. The sawdust enters a dryer and exits at 10% moisture content and 80°C. The heat that must be used in the drying block is extracted through a heat stream connected to a HEATER, where the gas stream enters, and cools down. Later on, the removed liquid water is mixed with the gas stream to cool it down due to the evaporation of water. The simulation will be accepted if the vapour fraction of the outlet gas stream is one, which corresponds to the evaporation of all water removed from the biomass. The Figure 9 presents this sequence.

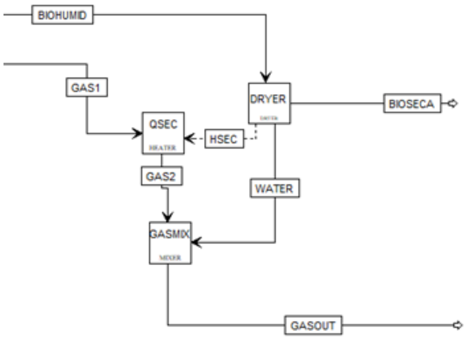


Figure 9 – Aspen blocks for dryer "Aspentech" model

The chosen dryer model was the first one, since it was the one recommended by Aspen.

5.2.4. Safety issues regarding storage

Dry sawdust when stored above certain temperature may incur in auto ignition or dust explosions. IEA Bioenergy (2017) states that typically dry biomass for pelletization is stored between 90°C and 180°C. A DESIGN-SPEC, SEGURAN, was created to ensure those conditions by the manipulation of the air inlet in the mixing chamber. Table 6 presents the air inlet flowrate for several exit temperatures.

Table 6 – Air flowrate as a function of the final temperature of the sawdust at the exit of the dryer

T (°C)	Air flowrate at the mixing chamber (kg/h)
90	109500
130	50500
170	29000

From the dryer simulation, using the first alternative method, a sensitivity analysis was performed by varying the amount of sawdust processed as well as the initial moisture content. Figure 10 presents the final dryer temperature and the water flow removed as a function of the amount of sawdust for an initial humidity of 40%. This figure also shows that for higher flowrates of sawdust (> 15 ton/h) it is no longer possible to dry, because the amount of water remains constant.

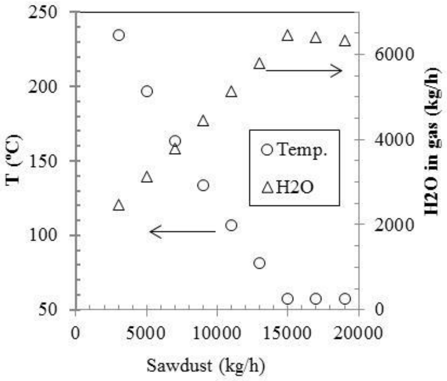


Figure 10 - Influence of the flowrate sawdust on the temperature and the water content in the outlet dryer gases (Sawdust moisture= 40%; Outlet dryer gases: flow rate = 50870 kg/h; temperature= 300ºC).

Figure 11 shows the final temperature of the dryer and the water removed as a function of the initial moisture of 7 ton/h of sawdust. In this case, it is possible to dry the sawdust independently of moisture content up to 55%.

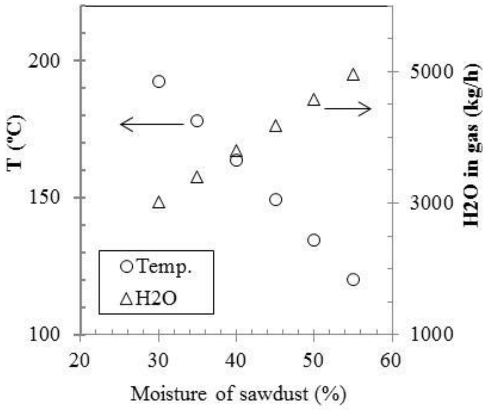


Figure 11 - Influence of the sawdust moisture on the temperature and the water content in the outlet dryer gases (Sawdust flow rate = 7000 kg/h; Outlet dryer gases: flow rate = 50870 kg/h; temperature= 300º C).

6. Biomass conversion processes

Several biomass conversion processes have been also analysed, such as electricity production, cogeneration and steam gasification.

6.1. Electricity production

The strategies to produce electricity consist in the production of superheated steam used in a set of turbines, sometimes with reheating in between. The gas stream outlet temperature at the boiler must be optimized to maximize the superheated steam production, but at the same time to generate a gas stream with a temperature, that allows its use in the dryer. Table 7 shows the results for several process conditions.

Table 7 – Simulation of electricity production using steam

P_{water} (bar)	$T_{steamboiler}$ (°C)	F_{water} (kg/h)	$P_{outlet\ turbine}$(bar)	Electricity (kW)	$T_{turbine\_out}$ (°C)
120	436,7	2500	2	448,6	122,1
80	436,7	2500	2	414,9	145,1
50	436,7	2500	2	374,7	173,3
80	801,6	2500	2	635,3	386,7
80	307,7	2750	2	392,3	120,2

6.2. Cogeneration

Cogeneration implies the use of process energy to produce both heat and electricity. This process needs hot water for greenhouses heating.

Three different integration scenarios were evaluated to simulate the cogeneration process, where hot water is produced through the outlet gases of the boiler or indirectly by the steam coming out of the turbine.

The first alternative assumes that steam, after expanding in a turbine at 2 bar, produces hot water to achieve the conditions to be used in the greenhouses.

The second scenario is similar to the first one, but uses an extraction turbine. A first turbine has an output at 5 bar, and a fraction goes to another turbine and expands to 0,3 bar. The 5 bar steam fraction enters a heat exchanger and heats the water for the greenhouses. This process is presented in Figure 12.

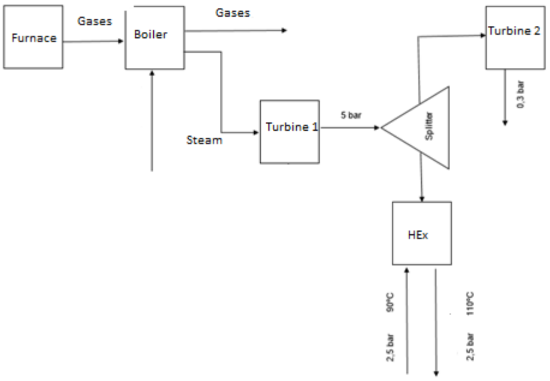


Figure 12 – Aspen diagram block for cogeneration alternative

The results for several split fractions are presented in Table 8.

Table 8 – Simulation of electricity production using steam

$T_{gasboiler}$ (°C)	$P_{1st\ turbine\_out}$ (bar)	Electricity (kW)	$P_{2nd\ turbine\_out}$ (bar)	Electricity (kW))	$F_{hotwater}$ (kg/h)
464	5	292,5	0,3	174	21000
464	5	292,5	0,3	149,1	28000
464	5	292,5	0,3	124,3	35000

The third alternative assumes that the exhaust gases coming from the furnace are used to produce superheated steam and consequently the gases are still used to produce hot water before entering in the mixing chamber.

A comparison between the three methods was made. The third one may result in larger corrosion problems due the direct contact between the combustion gas and the heat exchanger. Between the first and second alternatives, one must choose the one that adequate more to the user’s present needs: hot water or electricity. It must be noted that the second method needs a larger equipment invest, due to the extraction turbine.

7. Conclusions and future work

The present dissertation developed a simulation model in Aspen Plus of part of an industrial process of pelletizing, including a combustion unit, a gas-solid separation and drying operation. The available industrial data allowed a good comparison, namely in the combustion stage.

This model allows a simulation for the main unit operation in a pellets plant for different biomass feeds and different operational condition, without the intervention of the user.

Due to the untapped heat in the process, electricity generation and water heating operations were also studied to increase global efficiency.

A rice stem feed was used to develop a gasification simulation model. Due to the lack of industrial data for this process, a literature data was used in the different calculation steps.

As future work, there is a need for a deeper analysis of the results of the processes studied, comparison with industrial data, and also the development of a more detailed gasification model.

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