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Sugarcane bagasse gasification: thermodynamic modelling and analysis of operating effects in a steam-oxygen-blown fluidized bed using Aspen Plus^{TM}

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Sugarcane bagasse is an abundant agricultural residue derived from the sugar-alcohol industry, which is usually burned in boilers for power generation. However, this practice results in relatively low yields and ash production, requiring the investigation of novel methods of sugarcane bagasse conversion. In this context, gasification arises as a promising option: it is a thermochemical process that converts a wide range of carbonaceous resources into syngas, a gaseous mixture that mainly contains H_2, CO, CO_2, CH_4 and light hydrocarbons, and can be applied in the generation of heat, power, and chemicals. Gasification can be held in different gasifier configurations, but special attention is given to fluidized beds due to advantages such as feeding flexibility and scalability, high heat and mass transfer rates, and high reaction rates. Despite the given panorama, there is a lack of data in the literature of sugarcane bagasse gasification in bubbling fluidized beds operating with steam and oxygen as gasifying agents. To address this subject, this work performed a simulation of sugarcane bagasse gasification in a steam-oxygen-blown bubbling fluidized bed based on Gibbs free energy minimization using Aspen Plus^{TM}. With the proposed model, a 2^4 factorial design was conducted with the intent to study the influence of gasification temperature, pressure, biomass moisture content, and steam-to-biomass ratio (S/B) on syngas production. The obtained results have shown how different operating conditions and their interactions affect gasification exothermic and endothermic reactions and, consequently, compositions and performance indicators. Finally, the present work has demonstrated that sugarcane bagasse gasification is a potential and feasible process for clean energy production, contributing as an alternative for this agricultural waste use.

1. Introduction

Research in renewable energy sources is a topic that receives much attention due to the worldwide growing energy demand, as well as the need to reduce both greenhouse gas (GHG) emissions and the dependence on fossil fuels. In this sense, biomass feedstocks appear as a promising alternative owing to their low costs and abundance in many regions; to the possibility of producing a wide range of energy forms, such as heat, electricity or transportation fuels; and to its almost carbon neutrality, reducing GHG emissions (Akay and Jordan, 2011).
Sugarcane is the second most produced commodity crop worldwide (nearly 1.9 billion tonnes in 2016), being extensively produced in countries like Brazil, India, China, Thailand, and Pakistan (Food and Agriculture Organization of the United Nations, 2018). Sugarcane milling produces by-products such as sugarcane bagasse, an agricultural residue mainly burned in cogeneration systems to produce heat and electricity. However, bagasse burning results in low efficiencies (Modesto et al., 2016), which requires the study of more efficient methods of conversion of bagasse into energy.
Gasification is one of the most attractive options for biomass thermoconversion, and it is defined as the conversion of carbonaceous solids or liquids at temperatures of 600 – 1500 ºC under the presence of gasifying agents and oxygen feeds below oxidation stoichiometric values (Anukam et al., 2016). Gasification generates a

gaseous phase, known as synthesis gas or syngas, which is the main gasification product; a liquid phase, known as tar; and a solid phase, denominated as char (Molino et al., 2016). Syngas is mainly composed of H_2, CO, CO_2, and CH_4, and it can be used in low added-value applications, such as combustion in engines or gas turbines, as well as in high added-value uses, such as catalytic and biocatalytic processes to synthesize organic acids, alcohols, esters, and hydrocarbons (Bain and Broer, 2011).
Heretofore, most of the investigations on sugarcane bagasse gasification were directed to lower added-value applications, which are associated to obtaining low added-value syngas using cheaper gasifying media like air (Figueroa et al., 2017) or inert beds like sand (Sahoo et al., 2014). Moreover, no experimental investigations on bubbling fluidized bed gasification of bagasse at conditions that enhance syngas' compositions for higher added-value purposes have been found, which requires the evaluation of their potential via thermodynamic simulations. Given this panorama, this paper aims at studying, via simulation, the influence of different operational parameters on sugarcane bagasse gasification in a bubbling fluidized bed with steam and oxygen as gasifying agents, and olivine as bed, which are conditions that are suitable for obtaining higher-quality syngas mixtures. In order to achieve this goal, a simulation of the system was conducted based on Gibbs free energy minimization using Aspen Plus™, as well as a 2^4 factorial design to study the effects of gasification temperature, pressure, biomass moisture content, and steam-to-biomass ratio (S/B) on syngas compositions, H_2/CO ratio, cold gas efficiency (CGE), and equivalence ratio (ER) required to maintain gasification temperature.

2. Materials and Methods:

2.1 Simulation description

The simulation was performed in Aspen Plus V.8.6 and was based on some assumptions: simulation is zero-dimensional; the gasifier is isothermal and operates at steady state; pressure drops are neglected; char is composed of 100% carbon; ash is considered inert; all fuel-bound N_2, S, and Cl_2 are converted to NH_3, H_2S and HCl; drying and pyrolysis are instantaneous; tar formation is not considered; heat loss from the gasifier is neglected; and Peng-Robinson with Boston-Mathias modifications (PR-BM) was selected as the thermodynamic package (Doherty et al., 2013). The process flow diagram is shown in Figure 1.

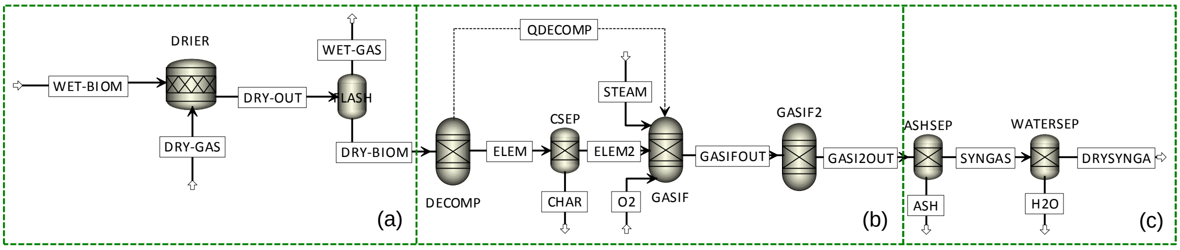

Figure 1: Process flow diagram of simulation: (a) biomass drying; (b) gasification; (c) ash and water removal.

In the flowsheet, the stream WET-BIOM corresponds to the wet bagasse, which is fed at 25 ºC, and corresponds to a non-conventional stream. The ultimate and proximate analyses of bagasse were inserted, as well as the feedstock higher heating value with HCOALGEN and DCOALIGT property methods to estimate the biomass enthalpy of formation, specific heat capacity, and density.
The blocks DRIER and FLASH correspond to the drying stage of the system (Figure 1 (a)). DRIER is an RStoic block to simulate the conversion of part of the biomass into water when in contact with a nitrogen or flue gas stream (DRY-GAS). FLASH is a FLASH2 type block to perform the separation between the dry biomass (DRY-BIOM) and the removed moisture content and drying media (WET-GAS). A design spec was set to vary the WET-BIOM flow rate so that the DRY-BIOM flow rate would be 20 kg/h. More details on how to setup the drying blocks are described elsewhere (Aspen Tech, 2013).
The blocks DECOMP, CSEP, GASIF AND GASIF2 correspond to the gasification stage (Figure 1 (b)). The block DECOMP is an RYield block to convert the non-conventional stream DRY-BIOM into conventional components, whose yields are set by a calculator block that makes use of the biomass' ultimate analysis data. The block CSEP separates part of the char, which is assumed to be entirely composed of carbon (C). The block GASIF is an RGibbs block that promotes the gasification between streams ELEM2, STEAM and O2. The stream STEAM consists in saturated water at saturation temperature, whereas the stream O2 consists in oxygen at 150 ºC. Both STEAM and O2 are fed at gasifier pressure. The gasification reactions, which are present in Table 1, were inserted in the GASIF block with zero temperature approach. The product of GASIF, that is, the stream GASIFOUT, enters the block GASIF2, which is also an RGibbs block, and has the function of adjusting the gas composition to experimental data, as proposed by Doherty et al. (2013), by restricting the equilibrium of reactions

R7 and R8 with temperature approaches. Finally, the separator ASHSEP simulates the removal of ash, whereas the separator WATERSEP simulates the removal of water from syngas (Figure 1 (c)).

Table 1: Gasification reactions.

Reaction number	Reaction	Reaction name	Heat of reaction[a] (MJ/kmol)
R1	$C + 0.5\,O_2 \rightarrow CO$	*Char partial combustion*	*-111*
R2	$C + 2\,H_2 \rightarrow CH_4$	*Methanation reaction*	*-75*
R3	$CO + 0.5\,O_2 \rightarrow CO_2$	*CO partial combustion*	*-283*
R4	$H_2 + 0.5\,O_2 \rightarrow H_2O$	*H_2 partial combustion*	*-242*
R5	$C + CO_2 \leftrightarrow 2\,CO$	*Boudouard reaction*	*+172*
R6	$C + H_2O \leftrightarrow CO + H_2$	*Water-gas reaction*	*+131*
R7	$CO + H_2O \leftrightarrow CO_2 + H_2$	*Water-gas shift reaction*	*-41*
R8	$CH_4 + H_2O \leftrightarrow CO + 3\,H_2$	*Steam-methane reforming*	*+206*
R9	$CH_4 + 2\,H_2O \leftrightarrow CO_2 + 4\,H_2$	*Steam-methane reforming*	*+165*

[a]Heats of reaction at 25 °C.

2.2 Simulation validation

Due to the lack of data of sugarcane bagasse gasification under the conditions studied in this paper, the simulation was validated with results of Miscanthus X Giganteus gasification in a steam-blown bubbling fluidized bed that uses olivine as bed material (Michel et al., 2011). Miscanthus was chosen because its proximate and ultimate analyses are similar to those of sugarcane bagasse, as demonstrated by other works (Leal Silva et al., 2017) and depicted in Table 2. After the validation of the simulation with Miscanthus results, sugarcane bagasse proximate analysis, ultimate analyses and higher heating value were inserted, as well as an O_2 stream (O2) to the gasifier GASIF to generate heat for the process, and a heat stream (QDECOMP).

Table 2: Proximate and ultimate analyses of feedstocks.

Proximate analysis (dry basis)	Miscanthus X Giganteus[a]	Sugarcane Bagasse[b]	Ultimate analysis (dry basis)	Miscanthus X Giganteus[a]	Sugarcane Bagasse[b]
Volatile matter (%)	*80.2*	*79.06*	*C (%)*	*47.1*	*46.96*
Fixed carbon (%)	*17.5*	*18.00*	*H (%)*	*5.38*	*5.72*
Ash (%)	*2.3*	*2.94*	*O (%)*	*46.946*	*44.05*
Moisture content (%)	*9.4*	*50.00*	*N (%)*	*0.44*	*0.27*
HHV (MJ/kg)	*n.d.[c]*	*18.5*	*S (%)*	*0.06*	*0.02*
			Cl (%)	*0.074*	*0.04*

[a]Michel et al. (2011); [b]de Medeiros et al. (2017); [c]not determined.

2.3 Influence of operating parameters

The influence of temperature, pressure, biomass moisture content, and steam-to-biomass ratio was evaluated both via an individual sensitivity analysis and via a 2^4 factorial design, as shown in Table 3.

Table 3: Operating conditions for sensitivity analysis and 2^4 factorial design.

Factor	Base case for sensitivity analysis	2^4 Factorial design	
		-1	+1
Temperature, T (°C)	*850*	*750*	*950*
Pressure, P (bar)	*1*	*1*	*15*
Moisture content, MC (%)	*10*	*10*	*30*
Steam-to-biomass ratio, S/B	*1.0*	*0.5*	*1.5*

The sensitivity analysis of each base case parameter was carried out to observe their effects on syngas compositions (H_2, CO, CO_2 and CH_4). The 2^4 factorial design analysis, on the other hand, was performed in the software Statistica 7.0 at a 99.0% confidence level to assess the effect of operating parameters on H_2/CO ratio, cold gas efficiency (CGE), and equivalence ratio (ER) requirements to achieve the desired gasification temperature. S/B and CGE are calculated as follows:

$$S/B = \frac{steam\ flow\ rate}{biomass\ flow\ rate} \qquad (1)$$

$$CGE = \frac{HHV_{syngas} \times dry\ syngas\ flow\ rate}{HHV_{biomass} \times dry\ biomass\ flow\ rate} \times 100\ \% \quad (2)$$

3. Results and discussion

Table 4 shows the conditions used in the validation run according to the work of Michel et al. (2011), as well as the experimental and simulated results. It can be seen that the simulated results are in good agreement with the experimental data, which indicates the simulation was successfully validated.

Table 4: Conditions used for simulation validation and obtained results.

Parameter	T (ºC)	P (bar)	S/B	H_2 (% dry vol.)	CO (% dry vol.)	CO_2 (% dry vol.)	CH_4 (% dry vol.)
Experimental	*880*	*1*	*1.1*	*45.89*	*22.04*	*7.71*	*24.35*
Simulated	*880*	*1*	*1.1*	*45.89*	*22.04*	*9.60*	*22.40*

Figure 2 shows the results of the influence of operating parameters on syngas composition obtained via sensitivity analysis.

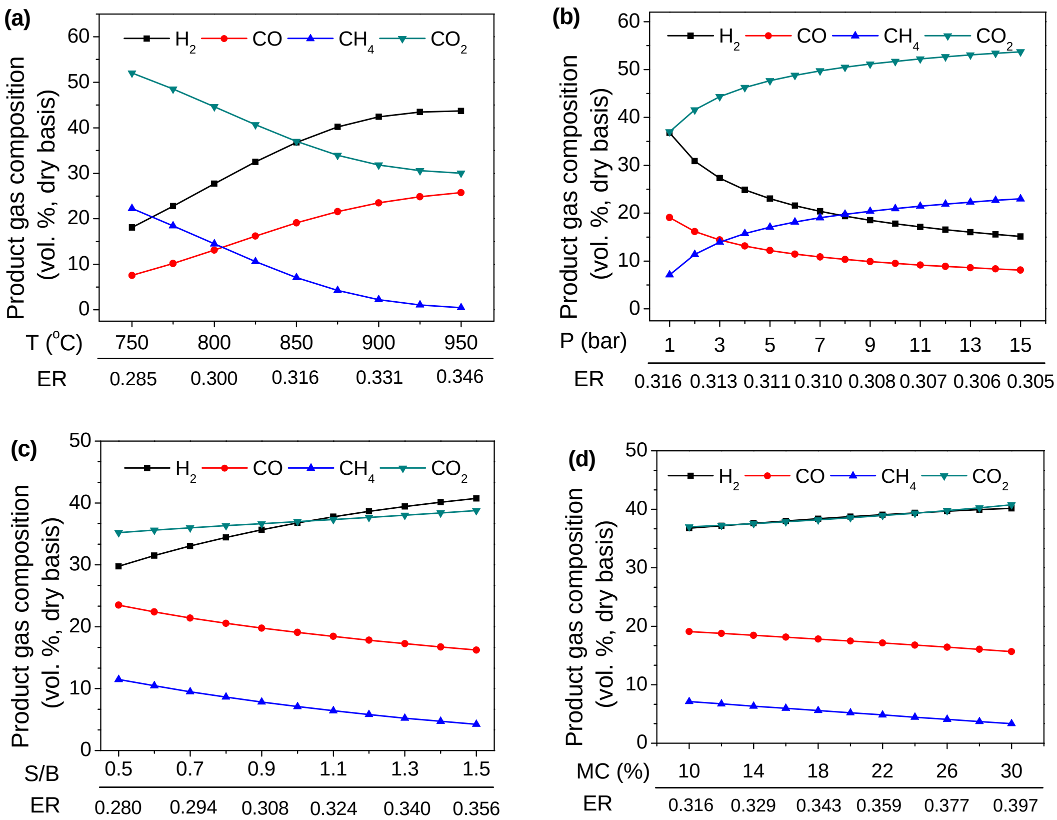

Figure 2: Sensitivity analysis - influence of (a) T, (b) P, (c) S/B, and (d) MC on syngas composition.

Figure 2 (a) demonstrates that temperature had a positive effect on H_2 and CO production, whereas it had a negative effect on CO_2 and CH_4 generation. This happened because, according to the Le Châtelier principle, a temperature increase in gas-phase systems will shift the chemical equilibrium to the side of reactants in exothermic reactions (R3, R4, R7), and to the side of products in the case of endothermic reactions (R5, R6, R8, R9). Figure 2 (b) shows that pressure, on the other hand, had a positive effect on CO_2 and CH_4 production, and a negative effect on H_2 and CO generation. In line with the Le Châtelier principle, a pressure increase will shift the equilibrium to the side with fewer molecules, that is, reactions R3 and R4 will be shifted towards the products, while reactions R8 and R9 will be shifted towards the reactants. Reactions R5, R6, and R7 were not affected by pressure since they are equimolar (Wan, 2016). Figure 2 (c) shows that steam injection into the gasifier favored reactions R7, R8, and R9, leading to H_2 and CO_2 formation and to CO and CH_4 consumption. Figure 2 (d), finally, evidences that, although moisture content is a form of water, it had a milder effect on syngas composition than saturated steam, as demonstrated by the smaller composition variations in comparison to steam (Doherty et al., 2013).

Figure 3 shows the pareto charts of effects of the factorial design analyses on CGE, H_2/CO, and ER.

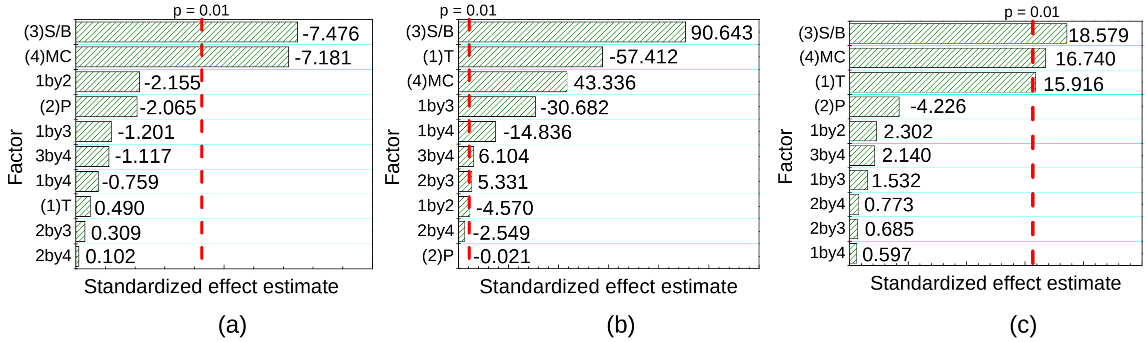

Figure 3: Pareto charts of effects of 2^4 factorial design analysis on (a) CGE, (b) H_2/CO, and (c) ER.

For the CGE analysis (Figure 3 (a)), steam-to-biomass ratio was the most significant factor, followed by moisture content. All statistically significant parameters had a negative effect on CGE. Since the dry biomass rate and the biomass HHV were held constant, all variations were due to the dry syngas rate and HHV, as per equation (2). CGE decreased with increasing S/B and MC because, although such variations generated a small dry syngas rate increase, a more pronounced syngas HHV decrease occurred due to a CH_4 composition decrease, as shown in Figures 2 (c) and (d). Temperature and pressure were not significant for a 99.0 % confidence level.

For the H_2/CO analysis, steam-to-biomass ratio was the most significant factor, which is in accordance with the results portrayed in Figure 2 (c). Steam had a positive effect on H_2/CO ratio, which demonstrates that it is a key factor for the adjustment of H_2/CO ratio for higher added-value downstream processes. Temperature was the second most significant parameter, presenting a negative effect. Although moisture content had a positive effect on H_2/CO ratio, it was milder than S/B, which is because moisture is less reactive than steam as presented by previous works (Doherty et al., 2013). In addition, higher moisture contents are usually associated to operational difficulties, as experienced by previous experimental works (Kaewluan and Pipatmanomai, 2011).

Steam-to-biomass ratio, moisture content and temperature had positive effects on the ER requirements to achieve the gasification temperature, which agrees with Figures 2 (a), (c), and (d).

All the obtained models for the analyses were considered statistically significant to the F-test with 99 % confidence, and some of the contour plots of the significant factors are presented in Figure 4.

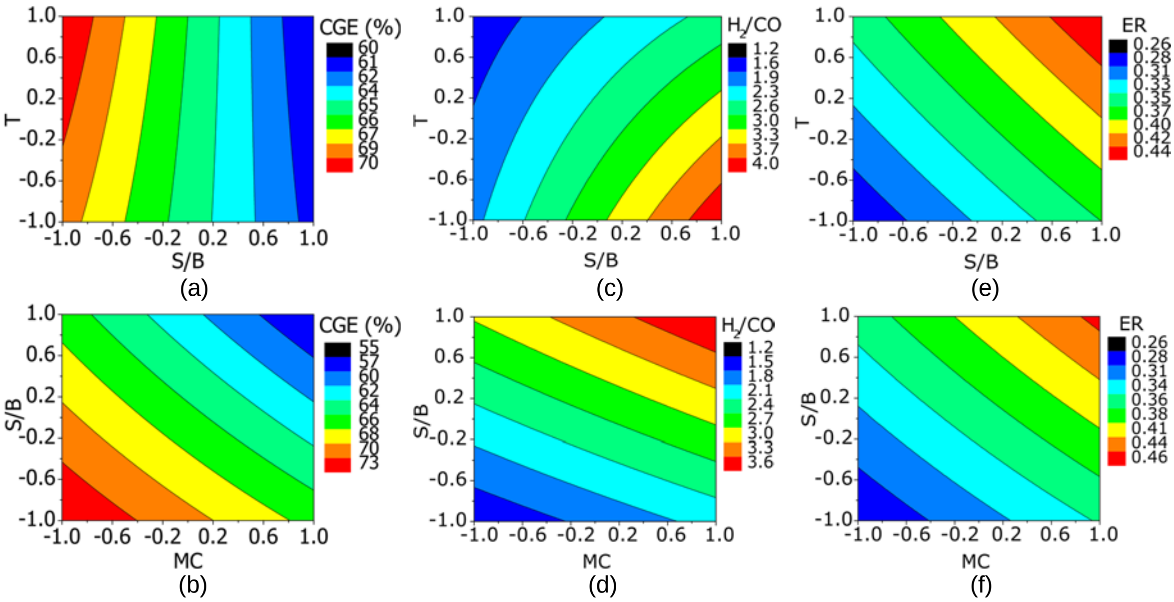

Figure 4: Contour plots of significant factors for CGE, H_2/CO and ER analyses.

The CGE contour plots (Figures 4 (a) and (b)) demonstrate that higher temperatures, as well as lower steam-to-biomass ratios and moisture contents contribute to higher CGEs. The H_2/CO ratio (Figures 4 (c) and (d)) was enhanced by lower temperatures, and higher steam-to-biomass ratios and moisture contents. Finally, to obtain lower ER requirements, temperature, steam-to-biomass ratio and moisture content must be as low as possible. Lastly, a comparison of Figures 4 (b), (d) and (f) shows that the conditions that lead to higher CGE and lower oxygen requirements (ER) are opposite to those that generate higher H_2/CO ratios. Nonetheless, since the goal of this work was to study conditions to obtain higher-quality syngas mixtures, H_2/CO ratio must be adopted as main criterion in future optimization works once it is the key performance indicator related to syngas quality.

4. Conclusions

This work studied the influence of different operational parameters of sugarcane bagasse gasification via thermodynamic simulations to evaluate the potential of a process with steam and oxygen as gasifying agents, and olivine as bed to produce higher added-value syngas. It was observed that the desired H_2/CO ratio is a key factor to define the operating parameters. Steam injection and temperature must be manipulated to adjust the syngas H_2/CO ratio, since the former contributes for H_2 production and the latter for H_2 and CO generation. However, such process choices may increase the energy demands (represented by higher ERs) and lower the process CGE. The results proved that bagasse gasification with steam-O_2 and olivine can be an attractive option to produce a wide quality range of syngas mixtures, being an interesting option for clean energy production.

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