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Comparative Performance Indexes for Ethanol Production Based on Autonomous and Annexed Sugarcane Plants

Pablo Silva Ortiz*, Rubens Maciel Filho

School of Chemical Engineering, University of Campinas (UNICAMP). Laboratory of Optimization, Design and Advanced Process Control (LOPCA). Av. Albert Einstein, 500. CEP 13083-852, Campinas-SP, Brazil.
pasilvaortiz@feq.unicamp.br

Future biomass conversion systems have to be developed using advanced technological routes in order to compete with fossil fuels, as well as to fulfill sustainability criteria. An attractive biomass feedstock for ethanol production is sugarcane, which is available in large amounts in several regions around the world. Although first-generation ethanol is a consolidated process, due to their large-scale production and tradition, there is still room for improved economic and environmental outcomes in the bioethanol industry.

Bearing this in mind, this work presents a detailed process design strategy for biomass to ethanol production (1st-generation ethanol technology) from sugarcane. The simulation processes were performed using Aspen Plus® software focus on the annexed plant (production of bioethanol and sugar) and autonomous distillery (only bioethanol is produced) systems. Furthermore, a performance comparison in terms of the exergy efficiency and the destroyed exergy rate as a metric conversion of the processes are determined. Hence, the techno-economic bottlenecks in bioethanol production are attained using the exergy as an index. In addition, the sustainability aspects involved in the process design of the sugarcane biorefineries was discussed through the renewability exergy index. The results showed that the annexed plant has a reduction in the process irreversibilities rate of 6 % approximately, and in the average unitary exergy cost rate of 10 % approximately, in comparison to the autonomous distillery. Even though the proposed methodology is applied to 1G ethanol, it may well suited for several bioprocesses as a tool to help in taking decisions regarding design as well as operational policy definitions.

1. Introduction

The first-generation (1G) bioethanol is at present produced commercially from edible crops using biochemical methods. Thus, more than the half of the world bioethanol production comes from sugar-containing crops, mainly sugarcane, sugar beets, and sweet sorghum (Ptasinski, 2015). These crops accumulate high amounts of sugars that can be directly extracted and fermented into ethanol, according to the technology. Sugarcane is so far the most efficient feedstock for bioethanol production, particularly due to low consumption of fossil energy during sugarcane processing (Ptasinski, 2015). In 2016, US and Brazil were the first and the second largest producers of ethanol in the worldwide, respectively. In the US, approximately 58 billion liters of ethanol were produced, primarily from corn starch using alcoholic fermentation (RFA, 2017). Otherwise, in the Brazilian scenario sugarcane is one of the most important industries in the national economy, which processes 670.6 million ton of sugarcane to 38.9 million ton of sugar and 28.276,4 thousand m³ of ethanol (BEN, 2017).

Application of the techno-economic approaches to assess the ethanol production from sugarcane is extensive research field around the world. In this respect, it must be underlined that several Brazilian institutions have been analysed different biorefineries configurations including the ethanol and sugar plants (Ensinas et al., 2009); (Pellegrini and Oliveira Jr., 2011), (Pina et al., 2014) as well as independent distilleries that focus on exclusively in the ethanol production (Dias et al., 2011). Regarding the exergetic assessment of these systems, it should be noted previous results reported in the literature in this field by Pellegrini et al., (2008), Ensinas et al., (2009); Pellegrini and Oliveira Jr., (2011), Modesto et al., (2016) and Pina et al., (2017).

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Furthermore, an extension of this approach that covers the integration of the first and second generation ethanol through the use of lignocellulosic materials in the supply/product chain has been realized looking for improve the ethanol production rate (Ensinas et al., 2013); (Dias et al., 2014); (Bonomi et al., 2016a).
This work deals with the biochemical method of ethanol production from sugarcane in a Brazilian biorefinery context. In addition, it presents an approach to the problem of exergy optimization of the biorefineries system. A general model to the autonomous distillery (1G-AUT) and to the ethanol and sugar production processes (1G-ANX) were developed based on data for typical plants, and an exergy analysis for both systems was performed.

2. Process description

Data for the autonomous distillery and the annexed plant processing 4 million tonnes of sugarcane per season recovering 50 % of sugarcane straw with 30 wt.% moisture are considered. The main considerations of the sub-systems process (Sugar extraction, Juice treatment and concentration, Fermentation, Distillation, Ethanol production, Sugar production, which involves the Crystallization and Drying steps) for typical factories in Brazil are described in Bonomi et al., (2016b). The summary of the main parameters adopted in the simulation models is indicated in Table 1.

Table 1: Main parameters used in the simulation models

Parameters	***Value***
Crushing capacity	4 million TC/year
Effective period of operation	200 days
Sugar extraction	
Efficiency of sugar extraction in the mills	96 %
Bagasse moisture	50 %
Cogeneration system	
Pressure of the boiler system	65 bar
Steam temperature	485 °C
Boiler efficiency (LHV basis)	87.7 %
Isentropic efficiency (Extraction-condensing turbine)	85 %
Energy demand of the process	30 kWh/TC

The processes for the sugarcane distillery and the annexed plant were separated into several control volumes.
Extraction System: In this process is obtained the bagasse, which represents a by-product in suitable condition for burning in the boilers. A comparison of milling and diffusion systems from sugarcane is presented in Palacios-Bereche et al., (2014).
Juice Treatment: In this step, the raw juice from the extraction system is treated to remove non-sugar impurities, using chemicals (*Sulfuric acid-*H_2SO_4*, Ammonium hydroxide-*NH_4OH *(nutrients), Phosphoric acid-*H_3PO_4*, Calcium Oxide-CaO*). During this process, the juice is heated using vegetable steam from the multiple-effect evaporator.
Sugar Production: In this stage, boiling, crystallization, and drying processes are carried out. The sugar solution is called molasses or syrup and is used to produce ethanol by fermentation. Sugar extracted by the centrifuges has high moisture level, being sent to drying before it is packed.
Ethanol Production: This block included the alcoholic fermentation, distillation, rectification and dehydration steps. The *Melle-Boinot* fermentation process is most commonly used in the distilleries in Brazil. The alcohol in the broth is recovered by distillation, which uses the different boiling points of the various volatile substances present to separate them (Pellegrini and Oliveira Jr., 2011). Since ethanol and water form an azeotrope with concentration around 95 wt%, conventional distillation is used to produce hydrated ethanol, but alternative separation processes must be used to produce anhydrous ethanol, including azeotropic and extractive distillation and molecular sieves (Dias et al., 2014).
Combined Heat and Power-CHP: This system is responsible for the electromechanical demands of the mill. Hence, the bagasse generated in the extraction step is sent to the utility plant to raise steam to be used in extraction-condensing turbine.

3. Methodology

Mathematical models are used to simulate the steady-state operation of plants producing ethanol, sugar, and electricity (annexed plant, 1G-ANX) and producing ethanol and electricity (autonomous distillery, 1G-AUT).

3.1 Modeling Approach

The sugarcane biorefineries were simulated to determine mass, energy, and exergy balances. Hence, the Eq(1), Eq(2) and Eq(3) show the expressions used to obtained these balances for a generic control volume (CV), respectively, where $\sum_{inlet} \dot{m}_i b_i$ represent the exergy of the process inputs ($\dot{B}_{inputs}$), $\sum_{outlet} \dot{m}_e b_e$ the exergy of the process output ($\dot{B}_{products}$), and $\dot{B}_{dest.}$ the exergy losses (Irreversibilities).

$$\sum_{inlet} \dot{m}_i = \sum_{outlet} \dot{m}_e \qquad (1)$$

$$\sum_{inlet} \dot{m}_i h_i + \dot{Q}_{CV} = \sum_{outlet} \dot{m}_e h_e + \dot{W}_{CV} \qquad (2)$$

$$\sum_{inlet} \dot{m}_i b_i + \dot{Q}_{CV}\left(1 - \frac{To}{T}\right) = \sum_{outlet} \dot{m}_e b_e + \dot{W}_{CV} + \dot{B}_{dest.} \qquad (3)$$

3.2 Process Simulation

The process simulation are carried out by the use of Aspen Plus® V8.6 software. Since processes streams in ethanol plants are complex multi-component/multi-phase behavior, the thermodynamic method used in the simulation was the non-random two-liquid (NRTL) model for the calculation of activity coefficients in the liquid phase, while ideal behavior was assumed in the vapor phase modelling in order to determine the thermo-physical properties of each flow present in the system. Alternatively, the NRTL-HOC (Hayden-O'Connell) method was used for vapor-phase calculation when the concentration of acetic acid and other carboxylic acids is significant, like on the fermentation and distillation steps, as recommended by Bonomi et al., (2016b). In the cogeneration system, an enhanced SRK equation of state (EOS) based on the semi-empirical Redlich-Kwong with Soave modifications was used, since it is adequate for high temperature gases. In addition, STEAMNBS method was used for the steam streams, once it accurately represent pure water and steam for a wide range of pressures and temperatures (Aspentech, 2012).

3.3 Exergy calculation

The exergy method, which combines the First and Second Law of Thermodynamics, was applied to assess the performance of the various components in the annexed plant and autonomous distillery. Exergy is defined as the maximum work that can be obtained by means of reversible processes from a thermodynamic system that interacts with the components of the environment until the dead state equilibrium is attained (Szargut et al., 1988). The thermodynamic properties of the streams and substances present in the processes are evaluated at ambient conditions (298.15 K and 1 atm). The exergy analysis throughout this work was conducted using the data of mass flow rate, temperature, pressure, enthalpy, entropy and composition of each stream obtained in Aspen Plus®. For convenience, the sum of physical and chemical exergy called thermal exergy (B_{th}) as indicated by Szargut et al. (1988) was used for the total specific exergy calculation. The physical and chemical exergy were determinate according to Eq(4) and Eq(5).

$$B_{ph} = H + H_0 - T_0(S + S_0) \qquad (4)$$

$$B_{ch} = \sum_i x_i b_i^{ch} + R_u T_0 \sum_i x_i ln \Upsilon_i x_i \qquad (5)$$

where x_i is the mole fraction of component i in the mixture, and b_i^{ch} is the standard chemical exergy. The b_i^{ch} of the compounds was estimated using Szargut et al., (1988), as indicated for lignocellulosic biomass in Silva Ortiz and Oliveira Jr., (2014); Silva Ortiz and Oliveira Jr., (2016). In addition, the b_i^{ch} for compounds not available in the specialized literature of the exergy field was calculated according to the technical fuels procedure based on net heating values and atomic ratios (Szargut et al., 1988).

3.4 Performance indexes

Since exergy can be considered as a quality measure of the products, by-products, and residues at environmental/system conditions, it serves not only for defining indicators to assess the performance of chemical processes, but also as an indicator of environmental impact. Several technical indexes were proposed to evaluate the performance of the sugarcane biorefineries based on thermodynamic indicators.

Energy efficiency η_E***:*** Is defined by the ratio between the useful output (products) and input (resources) of an energy conversion process, Eq(6).

Exergy efficiency η_B: Is the ratio between the exergy of the products (ethanol, sugar, and surplus electricity) and the exergy of the resources (sugarcane and straw), as indicated in Eq(7).

$$\eta_E = \frac{\sum(\dot{m} \, . LHV)_{products}}{\sum(\dot{m} \, . LHV)_{resources}} \qquad (6)$$

$$\eta_B = \frac{\sum \Delta\dot{B}_{out,products}}{\sum \Delta\dot{B}_{in,resources}} \qquad (7)$$

Renewability exergy index (λ): This indicator takes into consideration the exergy associated to the useful products ($B_{products/by\text{-}products}$) of a given energy conversion process, the destroyed exergy or total process irreversibilities ($B_{destroyed}$), the exergy associated to the fossil fuels (B_{fossil}) required, the needed exergy to disposal the wastes, and the exergy related with emissions, residues and not treated wastes (Oliveira Jr., 2013). Depending on the λ value obtained from Eq(8), it indicates that: *(i).* Processes with $0 \leq \lambda < 1$ are environmentally unfavorable, *(ii).* For internal and externally reversible processes with non-renewable inputs, $\lambda = 1$, *(iii).* If $\lambda > 1$, the process is environmentally favorable, and additionally, increasing λ implies that the process is more environmentally friendly, *(iv).* When $\lambda \rightarrow \infty$, it means that the process is reversible with renewable inputs and no wastes are generated.

$$\lambda = \frac{\Sigma \dot{B}_{\text{products}}}{\dot{B}_{\text{fossil}} + \dot{B}_{\text{destroyed}} + \dot{B}_{\text{deactivation}} + \dot{B}_{\text{disposal}} + \Sigma \dot{B}_{\text{emissions}}} \quad (8) \qquad BCO_{2\,EE} = \frac{\text{Global CO}_{2\,equivalent\ emissions}}{\text{B}_{\text{products}}} \quad (9)$$

CO_2 equivalent rate ($BCO_{2\,EE}$): This indicator represented the relation between the estimate global CO_2 equivalent emissions emitted in the atmosphere due to its operation and the exergy of the products ($B_{products}$) for each configuration, as shown in Eq(9).

4. Results

The findings of this study indicate the relationship between the exergy and the sustainability aspects involved in the process design of the 1G-AUT and1G-ANX ethanol plants. Table 2 reports the data sources used in each biorefinery configuration to determine the renewability exergy index (λ). It was found that the annexed plant scores better considering the performance indexes previous defined with respect to the autonomous distillery.

Table 2: Renewability exergy index for the annexed plant and the autonomous distillery

	1G-ANX	*1G-AUT*
B chemical inputs (Fossil) *[kW]*	*6720*	*3309*
Sulfuric acid (H_2SO_4)	975	1547
Ammonium hydroxide (NH_4OH)	907	1442
Phosphoric acid (H_3PO_4)	42	41
Calcium oxide (CaO)	4800	279
B products *[kW]*	*627.524*	574.669
B surplus electricity	154.865	154.627
B ethanol	264.756	420.042
B sugar	207.903	0
B by-products and residues *[kW]*	*47.121*	*71.285*
Filter cake	11.755	23.324
Vinasse	35.366	47.961
B emissions *[kW]*	*35.530*	*35.574*
B destroyed or Irreversibilities (I) *[kW]*	*888.629*	*941.485*
Renewability exergy indicator (λ)		
Considering only products	0.67	0.58
Considering products and by-products	0.72	0.65

It is important to note that the exergy values of the net CO_2 emissions was similar for both plants. Regarding the categories shown for the λ index, the results indicated that the biorefineries processes (1G-ANX and 1G-AUT) were categorized as environmentally unfavorable, which means that the exergy of the products could not be used to re-establish the environment to the conditions prior to the occurrence of the process. Also, when it is considered the exergy values of products and by-products of these configurations, then the renewability could not be guaranteed even for an alternative low-carbon fuel as sugarcane ethanol.

4.1 Exergetic analysis of a sugarcane-based biorefineries

Regarding the exergetic assessment of the 1G-AUT and 1G-ANX systems, an exergy analysis comparison based on technical data for typical first-generation plants is shown in Table 3. The traditional 1G Mill corresponds to an annex plant producing sugar and ethanol (with 50% of sugarcane used for sugar, 50% for ethanol). It was also included several configurations at the CHP unit (Back-pressure, Condensing/Extraction steam turbines-ST) for the steam generation at different levels. In addition, the relation between the exergy destroyed (*I or* $B_{dest.}$) and the exergy of the products (B_P) for these configurations were determinate. It is emphasized that the irreversibilities rate and the exergy efficiency were obtained applying the exergy balance expression introduce in Eq(3) and the efficiency performance index shown in Eq(7), when these criteria were not reported by the authors. In those cases, the specific exergy values of the inputs considered were:

Sugarcane 5130 kJ/kg, Straw 16725 kJ/kg, and Bagasse 9667 kJ/kg. Concerning the exergy of the products, it was adopted for the sugar 17479 kJ/kg and 27042 kJ/kg ethanol.

Table 3: Exergy analysis of the first-generation ethanol production plants

Description	***Configuration***	***Live Steam generation [bar, °C]***	***$\eta_{B\cdot}$ [%]***	***Bdest. [MW]***	***Ratio [I/Bp]***
[1] Rankine without straw *(Condensing ST)*	*1G-AUT*	80 / 500	44.59	389	1.24
[2] Base case *(Back-pressure ST)*	*1G-ANX*	22 / 300	36.10	470	1.77
[3] Case I *(Conf. I - Back-pressure ST)*	*1G-AUT*	100 / 530	35.65	378	1.32
[3] Case II *(Conf. I - Back-pressure ST)*	*1G-ANX*	100 / 530	40.11	386	1.20
[3] Case I-TI *(Back-pressure ST, thermally integrated)*	*1G-AUT*	100 / 530	33.85	296	1.09
[3] Case II-TI *(Back-pressure ST, thermally integrated)*	*1G-ANX*	100 / 530	38.10	273	0.89
[4] Base case - Ethanol distillery *(Hydrated ethanol without surplus electricity)*	*1G-AUT*	21 / 300	32.15	298	1.31
[4] Configuration A *(Hydrated ethanol and surplus electricity)*	*1G-AUT*	67 / 515	34.27	310	1.27
[4] Configuration B (*Electrification of the milling)*	*1G-AUT*	67 / 515	34.72	312	1.27
[4] Configuration C (*Harvest, condensing ST)*	*1G-AUT*	67 / 515	36.45	394	1.52
[4] Configuration D (*Harvest, electrification of the milling and condensing ST)*	*1G-AUT*	67 / 515	36.77	389	1.49
[4] Configuration E (*Harvest, Multiple effect distillation)*	*1G-AUT*	67 / 515	37.54	417	1.57
[5] Base case - Traditional Mill	*1G-ANX*	21 / 300	43.50	323	1.34
[5] BPST - Back-pressure ST	*1G-ANX*	67 / 515	45.60	316	1.22
[5] CEST - Condensing-Extraction ST	*1G-ANX*	67 / 515	44.40	354	1.32
[5] SuSC - Supercritical Steam Cycles	*1G-ANX*	292 / 590	50.00	322	1.06

[1]Modesto et al., (2016) [2]Ensinas et al., (2009) [3]Pina et al., (2017) [4]Pellegrini et al., (2008) [5]Pellegrini and Oliveira Jr., (2011).

In order to contrast the global performance of the 1G-AUT and 1G-ANX systems with the earlier findings reported in Table 3, the overall assessment for the sugarcane biorefineries focused on the technical, environmental and economic (exergetic base) issues is summarized in Table 4. It is noted that the $BCO_{2\ EE}$ index was calculated in terms of the product(s) considered in the analysis. Highlighting the decrease of this index for the 1G-ANX system in 57%, when it is designed the joint production of ethanol, sugar and electricity.

Table 4: Global performance of the sugarcane biorefineries

	1G-ANX	*1G-AUT*
Products		
Ethanol production [L/TC]	53.07	84.19
Surplus electricity [kWh/TC]	181.86	181.58
Sugar production [kg/TC]	50.28	0
Efficiencies		
Energy efficiency [%]	48.93	44.81
Exergy efficiency [%]	41.39	37.90
Average unitary exergy cost [kJ/kJ]	2.41	2.63
Destroyed Exergy		
Irreversibilities [kWh/TC]	961.27	1018.45
Specific destroyed exergy [kJ/kg]	3460	3666
Ratio [I/Bp]	*1.42*	*1.64*
CO_2 equivalent rate ($BCO_{2\ EE}$) [gCO_2/MJ product(s)]		
$BCO_{2\ EE}$ (*Product: Ethanol, EtOH*)	297.17	187.54
$BCO_{2\ EE}$ (*Products: EtOH + Electricity*)	187.50	137.08
$BCO_{2\ EE}$ (*Products: EtOH + Sugar + Electricity*)	125.38	137.08

5. Conclusions

The performance indexes allowed to determinate the overall assessment for plants producing ethanol, sugar, and electricity. It must be pointed out that the lignocellulosic material (bagasse and straw) in both configurations was addressed it for the cogeneration unit, looking for improving the electricity for the grid. Hence, this comparison also indicated that the main exergy losses take place in the sections that exhibit the largest irreversibilities, the cogeneration system, the juice extraction, and the ethanol fermentation.

The overall energetic/exergetic efficiency shown a better performance in the annexed plant than the autonomous distillery as a function of the destroyed exergy rate, highlighting for both plants the impact of the irreversibilities in the cogeneration system and its dependence on the performance of these biomass conversion technologies. Lastly, the exergy-based renewability indicator demonstrated that the sugarcane biorefineries were categorized as environmentally unfavorable. However, this calculation only referred to the industrial processing stage.

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