Life Cycle Assessment of Biobutanol Production Integrated to Sugarcane Biorefineries in Brazil

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Abstract

New sugarcane biorefinery routes considering the integral use of biomass have become more important to the strategic objectives of the bioenergy production expansion in Brazil, especially for diversifying and adding value to the sugarcane production chain. Among these new products, biobutanol has been increasingly investigated, mostly for its use as a fuel, since its energy density is greater than that of ethanol, but also to replace an established use as feedstock in the chemical industry. In view of the new green chemistry technological routes development, it becomes interesting and necessary assessing the viability of the butanol production from sugarcane. In this study, the sugarchemical route characterized by the fermentation of sugarcane juice was evaluated using the Life Cycle Asessment method considering arrangements for the process integration in the existing Brazilian sugarcane biorefineries: first and second generation using ABE fermentation (acetone-butanol-ethanol) with wild and genetically modified strains. The evaluation approach took into account the whole production chain, from the agricultural stage, through the transportation of sugarcane and vinasse, to the industrial process of biobutanol production and its use as liquid fuel for transport. The software package SimaPro and the CML 2 Baseline 2000 v2.05 method were used as tools for the environmental impact assessment. The life cycle inventories were obtained from literature and mass and energy balances taken from process computer simulation. Results showed that butanol produced from the lignocellulosic material (cane bagasse and straw) presents lower environmental impacts compared to first generation scenarios evaluated. As well as previous biofuels production assessment studies have already pointed out, the agricultural stage is the most relevant to the total environmental impacts in the butanol case. Nevertheless, the use of water, enzyme, equipment (carbon steel), and the emissions from the bagasse combustion could be highlighted as the most important in terms of environmental impacts for the industrial stage. Results for the productivity per tonne of sugarcane in first generation scenarios indicate that the efficiency of the ABE fermentation process needs to be improved so biobutanol could turn into an economic viable alternative. The production of second generation biobutanol, on the other hand, could be a viable alternative for the integral use of biomass adding value to the sugarcane production chain. Its analysis accounting for production and use as liquid fuel for transportation has shown that results are at the same level as the impacts related to ethanol from sugarcane, presenting advantages if compared with gasoline in terms of global impacts, such as global warming and ozone depletion potentials. Nevertheless, categories related to local impacts such as eutrophication and acidification potentials presented higher values for butanol in comparison with gasoline.

Keywords: *life cycle assessment, butanol, sugarcane, biorefinery*

1. Introduction

According to the International Energy Agency (IEA, 2011), the global production of biofuels – liquid and gaseous fuels derived from biomass – has been growing steadily over the last decade from 16 billion liters in 2000 to more than 100 billion liters in 2011. Currently, biofuels provide around 3 % of total road transport fuel globally (on an energy basis) and considerably higher shares are achieved in certain countries. Brazil, for instance, met about 23 % of its road transport fuel demand in 2009 with biofuels. By 2050, biofuels could provide 27 % of total transport fuel and contribute in particular to the replacement of diesel, kerosene, and jet fuel. The projected use of biofuels could avoid around 2.1 gigatonnes of carbon dioxides emissions per year when produced sustainably. Leite et al. (2008) state that Brazil may have an important role in fulfilling the future demand for biofuels, due to the available agricultural area and to the three-decade experience on the ethanol production.

The maintenance of the Brazilian leadership on biofuels production will require globally competitive research, development and innovation, and high technical and scientific levels in all the production chain. Therefore, the development of new technologies is fundamental to allow the full use of sugarcane to the production of ethanol, coproducts and derivatives in a more efficient and sustainable way, aggregating value to the production chain by means of the development of new products and processes. Moreover, it is expected that a further diversification of the product portfolio of the sugarcane biorefineries will improve their robustness against market fluctuations and expand the use of sugarcane.

Butanol produced from the fermentation of sugarcane juice or the catalysis of ethanol has the possibility of playing an important role on adding value to the sugarcane production chain. With a projected annual growth rate of 4.7 %, today's world market for the chemical (mainly in the USA, China and Europe) is approximately 2.9 million tonnes per year (Mascal, 2012). Most of the butanol currently produced is oil-based and main producers are BASF, a Dow Chemical Company and the Oxea Group (Yuan and Hui-Feng, 2012). Particularly in Brazil, half of the annual demand of 60 thousand tonnes is produced internally by Elekeiroz (ABIQUIM, 2011). In the same way that the butanol produced by the petrochemical route, biobutanol may be used as solvent in a series of chemical processes and presents great potential to be used as fuel. If compared to ethanol, butanol presents several advantageous characteristics if used as liquid fuel for transportation. For instance, its lower heating value (LHV) of 27.8 MJ/L is higher than that of ethanol (21.2 MJ/L) and closer to gasoline's (31.2 MJ/L) (Dürre, 2007), and it is a superior blend stock than can be used with gasoline, diesel, biodiesel, and ethanol. As a chemical, butanol and its derivatives are employed in the production of polymers, plastics, paints and chemical stabilizers (Mascal, 2012; Menon and Rao, 2012).

In view of its physical-chemical characteristics, its potential use as chemical product and as fuel, and the possibility of its production by green routes (from biomass), it becomes important assessing the viability of different biobutanol production routes. Several studies in literature have already evaluated sustainability aspects of sugarcane biorefineries in Brazil (Cavalett et al., 2012, Dias et al. 2012, Figueiredo and La Scala, 2011; Walter et al., 2011; Vries et al., 2010; Hoefnagels et al., 2010; Brehmer and Sanders, 2009; Luo et al., 2009; Ometto et al., 2009; Macedo et al. 2008; Smeets et al., 2008; Goldemberg, 2007; Macedo, 2005).

In this work, the sugarchemistry route for the production of butanol were evaluated in terms of environmental impacts, considering the different integration designs of this process in the existing Brazilian sugarcane biorefineries. The Life Cycle Assessment (LCA) methodology were used to determine the impacts generated during the whole production and use chain, and to make a comparison possible between the different technological scenarios considered in this work. This assessment has used an innovative framework, the so called Virtual Sugarcane Biorefinery (VSB), which is under development by the Technological Assessment Program of the National Laboratory of Science and Technology of Bioethanol (CTBE) (Bonomi et al., 2012; Cavalett et al., 2012; Dias et al., 2012).

The main objective of this work was to evaluate the major environmental impacts related to different scenarios of butanol production integrated to a sugarcane biorefinery: (i) routes/alternatives were defined; (ii) life cycle inventory was constructed; (iii) environmental impacts were assessed; (iv) production stages with the highest environmental impacts were identified; (v) sensitivity analyses were carried out to assess the influence of industrial inputs on the environmental indicators; (vi) the use of butanol as liquid fuel for vehicles was compared to gasoline and ethanol in terms of environmental impacts.

2. Methodology

2.1. The virtual sugarcane biorefinery

According to Cavalett et al. (2012), the virtual sugarcane biorefinery (VSB) is a novel framework that integrates computer simulation platforms with economic, social and environmental evaluation tools to assess technical and sustainability indicators of different sugarcane biorefinery alternatives or routes. The construction of this tool is directly focused on key scientific and technological aspects of future biorefineries, requiring the elaboration of mathematical models to be introduced in the simulation platforms. The term "virtual" refers to the fact that the evaluation tool may calculate/predict some parameters of the various production alternatives of the sugarcane biorefinery using a computer simulation, without the need of performing all tests at industrial scale. At the same time, "biorefinery" refers to the coproduction of biofuels for transportation, generation of bioenergy and chemical products with high market value provided by renewable biomass sources. The concept is analogous to a petrol refinery, which produces multiple fuels and products having oil as feedstock. The approach of the VSB has already shown positive results and presents great potential to be used in the assessment of sugarcane biorefineries alternatives (Cavalett et al., 2012; Dias et al., 2010; 2011; 2012).

2.2. Evaluated sugarcane industrial processing scenarios

Fig. 1 shows a block flow diagram representative for integrated first and second generation production. Dashed lines and boxes represent flows and processes that only occur on second generation scenarios. In annexed plants, a fraction of the sugarcane juice is used to produce sugar and the remaining sugarcane juice, together with molasses (concentrated residual solution obtained after sugar crystallization) are sent to the concentration of the sugarcane juice, which will then be used for the ethanol and butanol production in the fermentation step. The main products considered for the biorefinery in this study are sugar, ethanol, butanol, acetone, and electricity. Since the biorefineries in Brazil are energy independent (steam and electricity) by using sugarcane bagasse (obtained as a by-product in the mills) and straw for combustion, process steam consumption directly impacts the production of surplus electricity, which may be sold to the grid.

According to the current trend of new plants in Brazil, the cogeneration system of the biorefinery has a 90-bar pressure integrated boiler and steam condensing turbines. In first generation scenarios, all bagasse and straw are burned for the production of steam and energy, whereas in second generation scenarios, a fraction of the bagasse and straw is pre-treated (forming the pentoses liquor) and hydrolyzed (forming the glucose liquor). Details on the cogeneration and on the ethanol/sugar production processes may be found on previous studies (Dias et al., 2011; Cavalett et al., 2012). Information on the fermentation and distillation stages in the butanol plant, as well as the used microorganisms may be found on the work by Mariano et al. (2012a; 2012b).

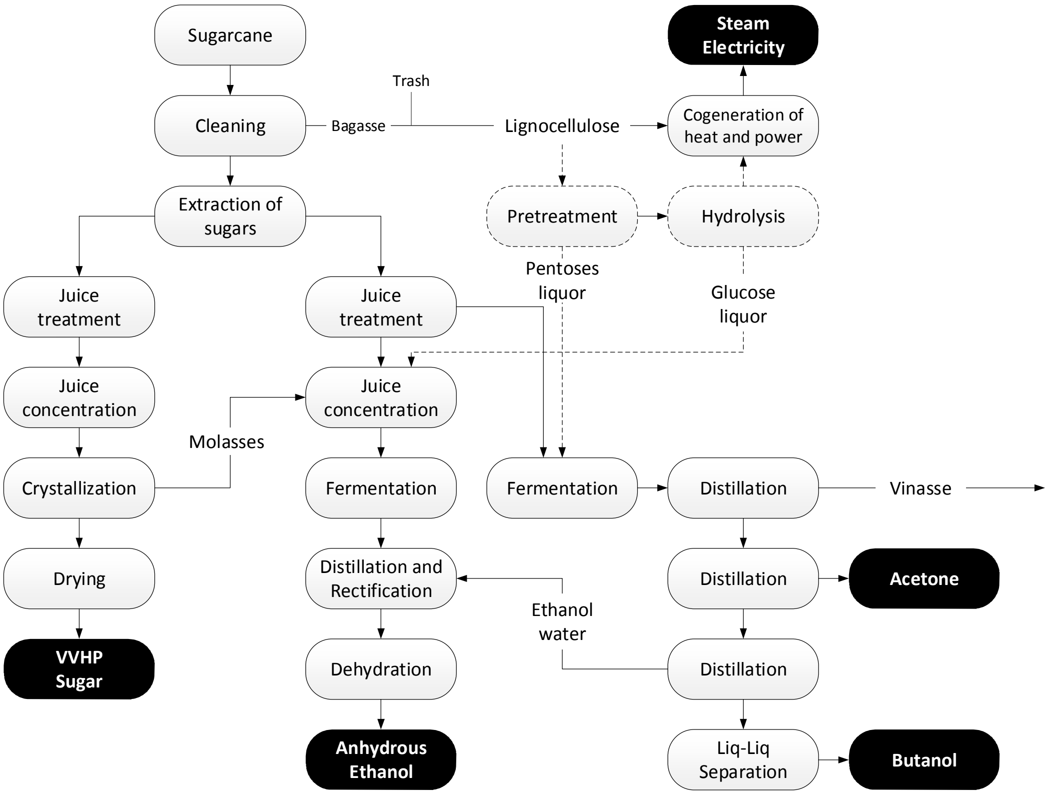

Fig. 1. Block flow diagram of integrated first and second generation production.

2.3. Life cycle assessment (LCA)

Within the concept of the VSB, the evaluation of environmental impacts is carried out by means of the LCA approach (ISO 14041, 1998; ISO 14040, 2006; ISO 14044, 2006). The life cycle of biofuels considers all stages from production and cropping of the vegetal biomass to the industrial process and transportation stages when necessary. The use as fuel for vehicles was also investigated within the LCA method in item **3.2** of this work.

The software package SimaPro and the CML 2 Baseline 2000 v2.05 LCIA method (described by Guinée et al. (2002)) were used as tools for the environmental impact assessment. The following impact categories were considered: abiotic depletion (ADP), acidification (AP), eutrophication (EP), global warming (GWP), ozone layer depletion (ODP), human toxicity (HTP), and photochemical oxidation (POP). According to the LCA methodology, allocation is required for multi-output processes as it is the case of a sugarcane biorefinery. In this study, economic allocation based on the market values of the products (**Table 1**) was applied, as described in the ISO documents.

Table 1. Average prices paid to the producer for products and derivatives.

Product	Price (US$)[A]	Reference
Sugarcane (ton)	27.26	6-year moving average prices (Dec 2011 values) Jan. 2003 to Dec. 2011 (UDOP, 2011)
VVHP Sugar (kg)	0.48	6-year moving average prices (Dec 2011 values) Jan. 2003 to Dec. 2011 (CEPEA, 2011)
Anhydrous ethanol (L)[B]	0.66	6-year moving average prices (Dec 2011 values) Jan. 2003 to Dec. 2011 (CEPEA, 2011)
Hydrated ethanol (L)[C]	0.59	6-year moving average prices (Dec 2011 values) Jan. 2003 to Dec. 2011 (CEPEA, 2011)
Electricity (MWh)	60.98	Average prices on renewable energy auctions in Brazil (values for 2011) (ANEEL, 2011)
Acetone (kg)	1.16	Considering its use as chemical (MDIC, 2011)
Butanol (kg)	1.03	Price considered proportional to anhydrous ethanol's energy content
Hexanol (kg)	3.29	Value updated for 2011 (ICIS, 2012)
Mixed alcohols (L)	0.91	Price considered proportional to anhydrous ethanol's energy content

[A]Prices in Brazil, considering an exchange rate of US$ 1.00 = R$ 1.673 (2011); [B]Density = 0.791 kg/L (ANP, 2011); [C]Density = 0.809 kg/L (ANP, 2011).

3. Results and discussion

Different scenarios of butanol production plants were evaluated. The main characteristics assumed for the biorefineries are displayed according to the scenarios presented in **Table 2**.

The quantities of the main inputs, outputs, and emissions for the industrial scenarios evaluated are shown in **Table 3**. Surplus electricity is similar for first generation scenarios (1G WS and 1G MS), due to the fact that all sugarcane bagasse and straw available are burnt. However, for the second generation scenarios considered in this work (1G2G MS and 1G2G WS), surplus electricity is much lower, since bagasse and straw are used both for the generation of electricity and the production of the liquors of pentoses and glucose. In second generation biorefineries, the maximum possible amount of lignocellulose is used for butanol production, but simultaneously power generation must comply with the process energy demand.

It is also possible to visualize in **Table 3** that considered scenarios generate different amount of vinasse from the distillation processes at the butanol plant. The fact is worth mentioning, because this vinasse is considered to be applied on the field, therefore, reducing the need for external fertilizers (mainly potassium) and affecting the environmental impacts.

Table 2. Description of the scenarios evaluated.

Scenarios	Description
1G2G WS	First generation annexed distillery with 50 % of the juice to the production of ethanol and 50 % to the production of sugar, integrated to the second generation (bagasse and straw) with the production of butanol from pentose fermentation by wild strain (*Clostridium saccharoperbutylacetonicum* DSM 2152)
1G WS	First generation optimized annexed distillery with 50 % of the juice to the production of ethanol, 25 % for the production of sugar and 25 % for the production of butanol by wild strain (*Clostridium saccharoperbutylacetonicum* DSM 2152)
1G2G MS	First generation annexed distillery with 50 % of the juice to the production of ethanol and 50 % to the production of sugar, integrated to the second generation (bagasse and straw) with the production on butanol from pentose fermentation by mutant strain (*Clostridium beijerinckii* BA 101)
1G MS	First generation optimized annexed distillery with 50 % of the juice to the production of ethanol, 25 % to the production of sugar and 25 % to the production of butanol from pentose fermentation by mutant strain (*Clostridium beijerinckii* BA 101)

Table 3. Inputs, outputs, and emissions for the industrial processing scenarios evaluated (per 1000 kg of sugarcane processed)

Scenarios	1G2G WS	1G WS	1G2G MS	1G MS	Unit
Products					
Anhydrous ethanol	51.97	36.85	52.26	36.85	kg
VVHP Sugar	51.13	25.54	51.13	25.54	kg
Electricity	90.55	169.81	90.61	169.87	kWh
Vinasse from ethanol process	720.14	509.27	724.99	509.27	kg
Filter cake mud	35.45	29.74	35.45	29.74	kg
Ashes	6.95	9.44	6.97	9.44	kg
Acetone	1.73	2.32	1.48	2.58	kg
Butanol	3.63	6.65	5.94	10.54	kg
Vinasse from butanol process	409.15	676.36	341.59	529.17	kg
Inputs					
Sugarcane	1000	1000	1000	1000	kg
Sulfuric acid	301	214	303	214	g
Lubricant oil	0.013	0.013	0.013	0.013	kg
Enzyme cellulase	0.85	0.00	0.84	0.00	kg
Water	2288.75	1500.00	2277.98	1500.00	m^3
Calcium hydroxide (lime)	1.35	1.21	1.35	1.21	kg
Zeolites	21.17	15.01	21.29	15.01	g
Inorganic chemicals	7.66	7.41	7.67	7.41	g
Equipment (carbon steel)	3.59E-01	2.68E-01	3.56E-01	2.41E-01	kg
Equipment (stainless steel)	1.98E-02	2.22E-02	1.90E-02	1.49E-02	kg
Industrial buildings and yards (concrete)	2.50E-04	1.47E-04	2.84E-04	1.34E-04	m3
Office and lab buildings (steel construction)	9.96E-05	5.86E-05	1.13E-04	5.33E-05	m2
Emissions to the air					
Ethanol plant					

Ethanol from distillation	0.11	0.08	0.11	0.08	kg
Carbon dioxide, biogenic from fermentation	53.79	37.73	53.70	37.73	kg
Bagasse combustion					
Carbon dioxide biogenic	242.25	318.35	242.83	318.35	kg
Carbon monoxide	158.15	214.81	158.57	214.81	g
Nitrogen oxides	157.35	213.72	157.77	213.72	g
Dinitrogen monoxide	8.69	11.80	8.71	11.80	g
Sulfuric oxides	8.44	11.47	8.47	11.47	g
Methane	65.17	88.53	65.35	88.53	g
Volatile organic compounds	11.00	14.94	11.03	14.94	g
Particulates <10μm	178.33	242.22	178.80	242.22	g
Particulates <2.5μm	89.16	121.11	89.40	121.11	g
Butanol plant					
Carbon dioxide, biogenic	10.31	28.14	10.53	18.73	kg
Acetone	18.1	23.1	15.8	25.8	g
Hydrogen	230	230	309	371	g

3.1. Life cycle assessment

Fig. 2 shows the comparative environmental impact scores for the butanol production in different industrial configurations. The values include the impacts from the agricultural phase, through the transport of sugarcane, to the industrial conversion in the biorefinery. In general, results show that second generation scenarios (1G2G WS and 1G2G MS) presented lower environmental impacts than first generation scenarios (1G WS and 1G MS), except for the POP category. In spite of these results, it is worth noticing from **Table 3** that 1G2G WS and 1G2G MS produce half the quantity of butanol per tonne of sugarcane in comparison with their respective first generation scenarios, since only the pentoses liquor is used as feedstock for butanol production in the second generation scenarios investigated in this work. It is also important to mention that analyzing 1G MS, it becomes clear that ethanol production is way higher (36.85 kg/TC) than butanol's (10.54 kg/TC), although the same amount of sugarcane juice is used as feedstock for the ethanol and butanol plants. This discrepancy is related to shortcomings/low efficiency of the ABE fermentation process that produces butanol along with ethanol and acetone. This process is still in research and development stage with the objective of improving the conversion of glucose to butanol and its titer/purity in the final broth, testing recovering techniques, enhancing the microorganism tolerance to solvents, and speeding up the process. According to Garcia et al. (2011), these enhancements may eventually improve the economics of the butanol production.

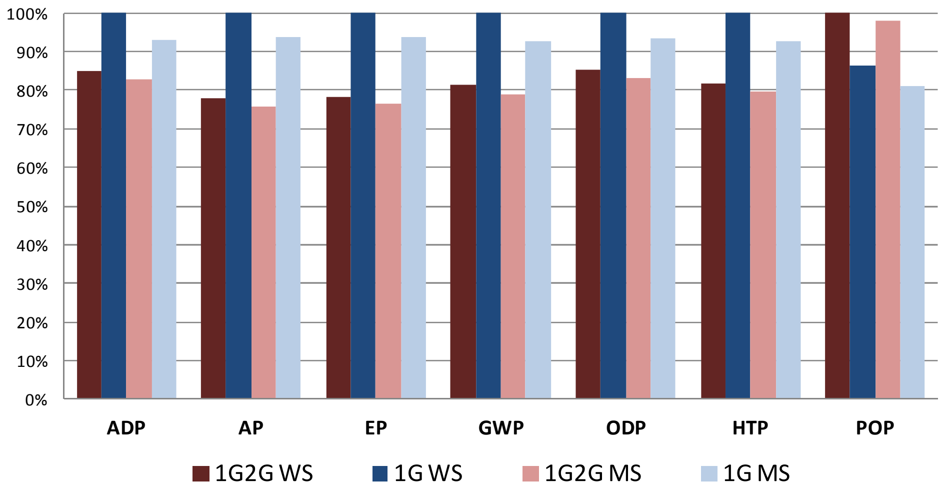

Fig. 2. Comparative environmental impact scores for butanol production chain.

Similarly to results obtained for the production of ethanol in first generation biorefineries in Brazil by Cavalett et al. (2012), the most impacting step for the butanol production chain is the sugarcane agricultural production. Therefore, the influence of different industrial configurations is diluted when the full sugarcane chain is considered. The only exception in this case is the POP category, in which most of the environmental impact is related to the industrial stage due to the direct emissions of gaseous ethanol during the distillation phase at the ethanol plant. **Fig. 3** shows comparative environmental impacts scores for the inputs used in the industrial processing stage of 1G2G MS scenario. In general, the use of water, enzyme, equipment (carbon steel), and the emissions from bagasse combustion could be highlighted as the most important in terms of environmental impacts for the industrial stage.

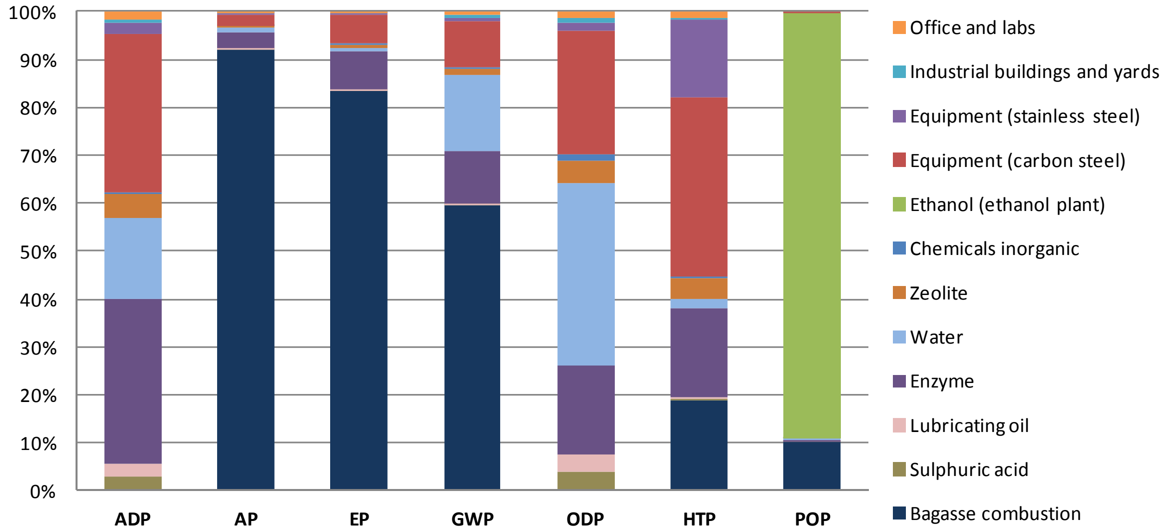

Fig. 3. Comparative environmental impacts scores for the inputs used in the industrial processing stage of 1G2G MS scenario.

Fig. 4 presents the comparative environmental impacts scores for the production of biobutanol only considering the industrial biorefinery conversion stage of the scenarios evaluated. It is possible to verify that the second generation scenarios present the highest impacts for ADP, ODP, HTP, and POP categories, due to the greater use of sulfuric acid, water, and cellulase, compared to the first generation scenarios. Despite this fact, the discrepancy do not reflect on the impacts related to the full production chain (**Fig. 2**), because as it has already been stated, impacts related to the agricultural stage are much higher than those from the industrial stage. Furthermore, second generation scenarios (1G2G WS and 1G2G MS) produce a smaller amount of butanol per tonne of sugarcane (approximately half of the quantity produce from the corresponding first generation scenarios, 1G WS and 1G MS) (**Table 3**), because only the pentoses liquor is used for the production. As a consequence of the reduced butanol production, there is a smaller allocation of the impacts from the agricultural stage for these scenarios than for the first generation ones.

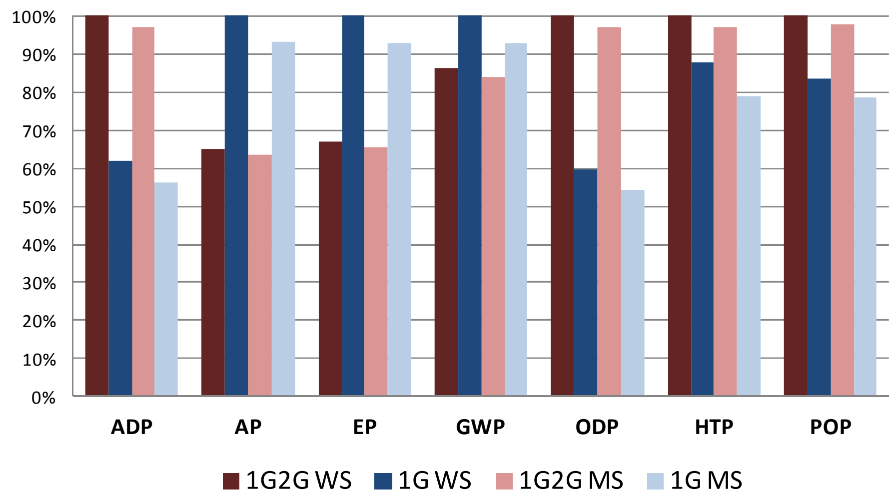

Fig. 4. Comparative environmental impact scores for the industrial stage of butanol production.

3.2. Butanol as liquid fuel

With the results obtained in this work for the butanol production from sugarcane, it was also possible to compare the environmental impacts with other fuels (and biofuels) in relation to their use as liquid fuel for vehicles. Since the energy contents of the fuels investigated at this item are different, and therefore, the amount of fuels used for each type of engine considered, the assessment must account not only for the use stage, but also for the whole production chain. The energy efficiency of engines were estimated for gasoline (3.46 MJ/km), ethanol (3.09 MJ/km), and flex (2.74 MJ/km) having as reference data from the Brazilian Ministry of Environment (MMA, 2011). The engine's efficiency is considered not to change as function of the type of fuel used. For example, a vehicle powered by a flex engine will have an energy efficiency of 2.74 MJ/km, whether it is powered by gasoline, ethanol, or butanol. By means of the engine's efficiency and the energy content of each type of fuel, it was possible to calculate its amount per kilometer. The energy contents considered were the following: hydrated ethanol (26.38 MJ/kg); gasoline C (43.54 MJ/kg); and butanol (34.32 MJ/kg) (ANP, 2011; Dürre, 2007).

Fig. 5 illustrates the comparative environmental impacts scores per kilometer for vehicles powered by three types of engines (flex, ethanol dedicated, and gasoline dedicated) according to each energy demand established by the MMA (2011) and considering the whole life cycle of the (bio)fuels evaluated. As it can be seen from the graphs, the use of gasoline presents the highest impacts for global categories such as ADP, GWP, and ODP. On the other hand, biofuels (ethanol and butanol) present the highest values for local environmental impacts such AP and EP, mainly due the use of chemicals and fertilizers in the agricultural stage of production. Therefore, having in sight all the evaluated categories, it is not possible to assert which type of fuel is more environmental friendly.

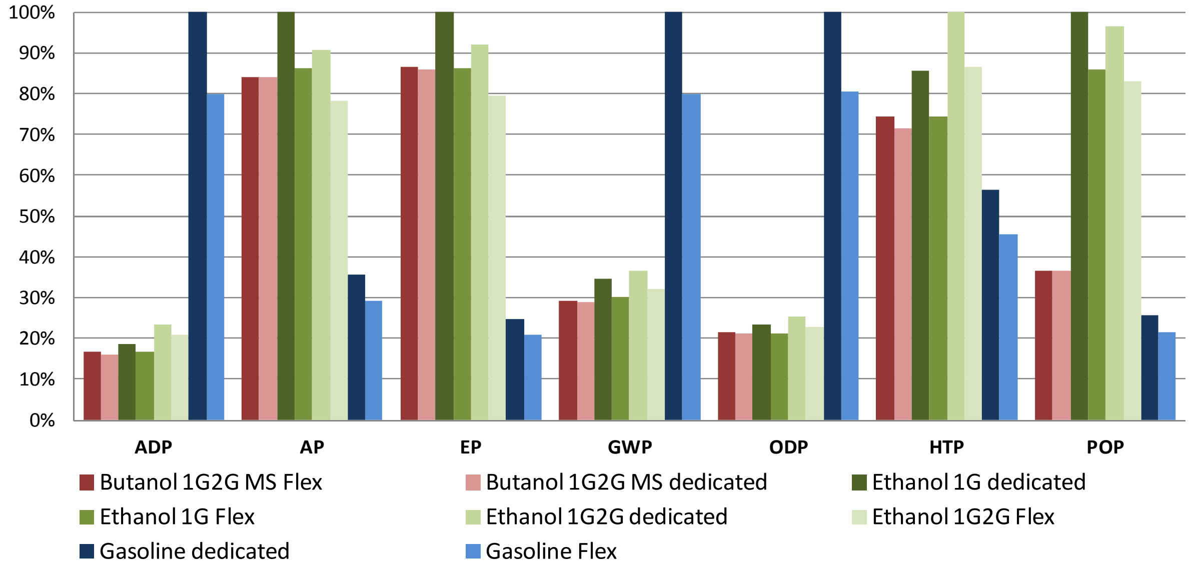

Fig. 5. Comparative environmental impacts scores per kilometer for a vehicle powered by: flex engine using butanol (1G2G MS), ethanol (1G and 1G2G from Dias et al., 2012), and gasoline (gasoline C); ethanol dedicated engine (1G and 1G2G from Dias et al., 2012); and gasoline dedicated engine (gasoline C) and butanol (1G2G MS).

3.3. Sensitivity analysis

Sensitivity analysis was carried out with the objective of measuring the environmental impacts as function of changes on the amounts of inputs used at the butanol production industrial stage. Second generation butanol production with ABE fermentation by mutant strain (1G2G MS) was selected for this analysis, since this scenario presented the best environmental results as shown in **Fig. 2**. Three environmental impact categories were selected for the evaluation: EP for representing local impacts, HTP for being related to human health, and GWP for representing global impacts. **Fig. 6** shows that EP presented the highest variation as function of the water use; HTP category is more sensitive to variations on the use of equipments (carbon steel); whereas lime has the biggest influence on the GWP category.

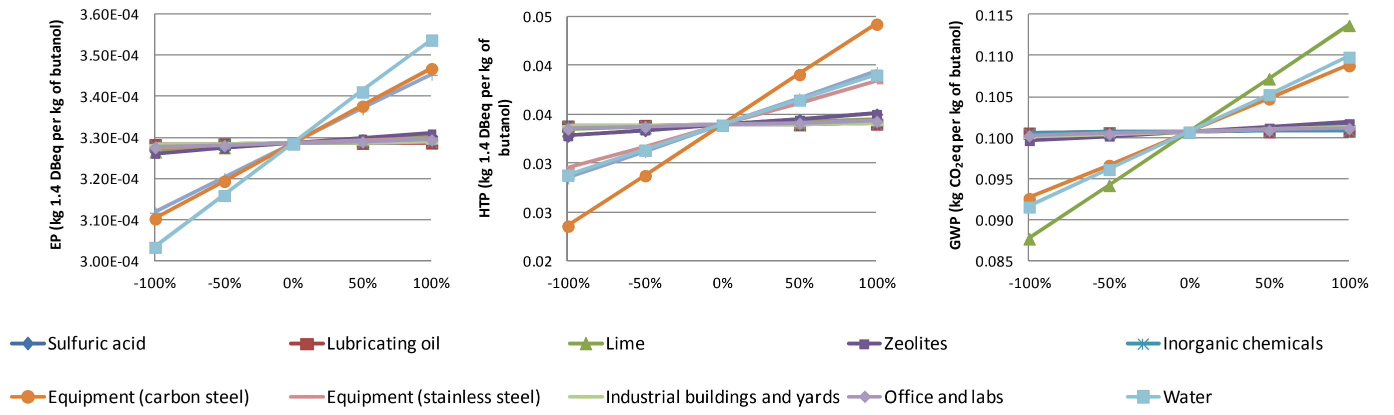

Fig.6. Sensitivity analyses of eutrophication potential (EP), human toxicity potential (HTP), and global warming potential (GWP) for the 1G2G MS scenario.

4. Conclusions

The production of butanol with pentoses liquor fermentation by mutant strain (1G2G MS) presented the lowest environmental impacts per kilogram of butanol produced among the scenarios evaluated. In the performed analysis, it became clear that the agricultural stage is the most relevant from the environmental standpoint for all biobutanol production chain. Nevertheless, the use of water, enzyme, equipment (carbon steel), and the emissions from the bagasse combustion could be highlighted as the most important in terms of environmental impacts for the industrial stage.

Results for the productivity per tonne of sugarcane in first generation scenarios (1G MS and 1G WS) indicate that the efficiency of the ABE fermentation process needs to be improved so that biobutanol could turn into an economic viable alternative. The production of second generation biobutanol, on the other hand, could be a viable alternative for the integral use of biomass adding value to the sugarcane production chain. Its analysis accounting for the production and use as liquid fuel for transportation has shown that results are at the same level as the impacts related to ethanol from sugarcane, presenting advantages if compared with gasoline in terms of global impacts, such as global warming and ozone depletion potentials. Nevertheless, it is worth mentioning that categories related to local impacts such as eutrophication and acidification potentials presented higher values for butanol in comparison with gasoline.

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