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Computer-Aided Environmental Evaluation of Bioethanol Production from Empty Palm Fruit Bunches using Oxalic Acid Pretreatment and Molecular Sieves

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This work evaluates the environmental performance of the bioethanol production process from the rachis of palm, through the route that includes Saccharification and Simultaneous Cofermentation (SSCF), as well as the dehydration by molecular sieves. The evaluation was carried out using the computer tool based on the waste reduction algorithm (WAR algorithm), quantifying the potential impacts generated (PEI) and classifying them into 8 different categories (four global and four toxicological). From the results obtained, the process studied transforms high power flows of PEI into output products of lower PEI, which is confirmed by the fact that the values of potential impacts generated are negative. Waste streams contribute greatly to the generation of potential impacts and different ways of exploiting these streams were explored. In addition, it was found that this process consumes less energy compared to other processes using the palm spine as a raw material, such as hydrogen extraction.

1. Introduction

The increase in energy demand has motivated the search for alternatives for obtaining energy from unconventional, environmentally friendly and economically sustainable sources. The production of bioethanol from lignocellulosic biomass is a promising alternative. However, it is necessary to evaluate the environmental impacts of this type of process from the conceptual design stage. Currently, the use of ethanol as a fuel is of special importance not only to reduce dependence on oil and face the energy crisis, but also as an effective way to contribute to the reduction of the great environmental impact generated by oil-based fuels (Montoya et al., 2006). Although almost all of today's fuel ethanol is generated from edible sources (sugars and starch), residual lignocellulosic biomass (LCB) has attracted much attention in recent times (Zabed et al., 2016).

In countries such as Malaysia and Indonesia, around 1 Mt of empty fruit bunches are wasted each year by the palm oil industry (Truong et al., 2014); this becomes a propitious space for the exploitation of this residual biomass, and the palm oil industry is very prosperous in tropical countries such as Colombia. Ethanol from palm rachis has become a very attractive option, mainly because of its ease of transportation, its renewable nature and its relatively uniform distribution throughout the world. On the other hand, environmental legislation has forced industries to comply with certain standards of clean production with the objective not only of achieving sustainable development, but also of contributing to the reduction of environmental pollution from the conceptual design of processes. The concept of implementing pollution prevention techniques in process design is not new; however, it has received more attention in recent years (Young et al., 1999). The waste reduction algorithm is presented as a useful and practical methodology to evaluate the environmental friendliness of a process. The PEI balance quantifies the impact of these pollutants on a process. Ultimately, the PEI balance is a quantitative indicator of the environmental compatibility or hostility of a manufacturing process (Young et al., 1999).

The WAR algorithm methodology, developed by the National Risk Management Research Laboratory of the US Environmental Protection Agency (EPA), proposes to add a conservation relationship on the PEI based on the input and output impact flows of the process (Montoya et al., 2006). It is understood as PEI, the possible effect that an amount of matter or energy could have when discharged out of the process. The WAR algorithm handles

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two kinds of indices to evaluate the environmental impact of a chemical industry. The first class measures the IMP emitted by the process and the other measures the generation of IMP in the process. Two main indices are defined within each class: those of total output impact (expressed as impact potential per unit of time) and those of impact per mass of product (Montoya et al., 2016).

Through this research work, it is intended to show the results obtained by carrying out the environmental analysis of the bioethanol production process through this algorithm, evaluating the global and toxicological implications of the currents of this process and visualizing possible solutions to achieve a better optimization of it through process integration techniques.

2. Materials and methods

2.1 Process description

The conversion of palm rachis into ethanol consists of several stages, as shown in Figure 1, each with characteristics, which make the process more profitable and efficient. The biomass (10,000 kg/h), after going through a previous drying process to reduce its humidity, is fed to a grinding stage (stream 1), with the aim of reducing and adapting its size. Then the raw material goes to an acid pretreatment stage (stream 2), which was made with oxalic acid (stream 3), in this stage a reaction occurs, and its main objective is to solubilize the hemicellulose that retains the cellulose forming a cellulose-hemicellulose chemical complex (Zabed et al., 2016), this complex is encapsulated by lignin, hindering the hydrolysis and subsequent formation of fermentable sugars. This is one of the most critical and costly steps in the process of converting Biomass to alcohol. For the biomass to be fermented, it must go through a process known as hydrolysis (stream 4) with sulfuric acid (stream 5), at this stage the polymeric sugars (hemicellulose and cellulose) are reduced in monomeric sugars. These sugars are passed through a neutralization stage with calcium hydroxide where the formation of calcium sulphate occurs.

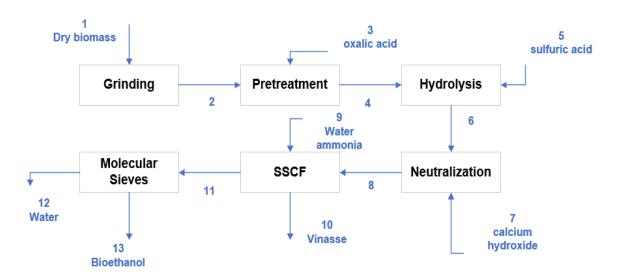


Figure 1: Block diagram of Production of Bioethanol from Palm Rachis

In the present study, the process analysis was carried out by means of the simultaneous saccharification route of cellulose and hemicellulose and co-fermentation of glucose and xylose (SSCF) in order to apply the concepts of process integration; which is characterized by having high ethanol yields and low production costs due to the simultaneous conversion of sugars. The challenge as such is to find a microorganism capable of supporting the conditions of saccharification and fermentation at the same time. However, in this case, we simply seek to analyse how much this configuration determines simultaneously the environmental impacts of the process studied. Finally, the mixture is passed through molecular sieves, with the aim of obtaining a higher purity ethanol, at the end, 1, 690 kg/h of bioethanol (stream 13) are obtained from this assembly.

2.2 Environmental assessment using WAR algorithm

For environmental evaluation of the bioethanol production process from palm rachis, the waste reduction algorithm (WAR GUI) was selected using the WARGUI software. This tool introduces the concept of Potential

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Environmental Impact (PEI) and allows to evaluate it in different categories of impacts, divided into two groups: atmospheric and toxicological; It also has the capacity to indicate how fast the environmental impact of the process could be in the environment, which cannot be determined with other methodologies as Life Cycle Assessment (LCA) (Herrera et al., 2017). The WAR algorithm relates the PEI to the flow of an environmental impact across the boundaries of the system, as a consequence of the mass and energy that crosses these limits and handles two kinds of indices to assess the environmental impact of a chemical industry, the first class measures the PEI emitted by the process and the other measures the PEI generated. Within each class, two indices are defined: total output impact indices (expressed as impact potential per unit of time) and impact indices per product mass. The main objective of the PEI output is to answer questions about the external environmental efficiency of the process, that is, the capacity of the process to obtain final products at a minimum discharge potential. Regarding the PEI generated its importance is to know the internal environmental efficiency of the PEI is calculated using Eq(1), the Total mass output rate is calculated by Eq(2), the Total generation rate is calculated by Eq(3), and the Total mass generation rate is calculated using Eq(4).

$$\dot{i}_{out}^{(t)} = \dot{i}_{out}^{(cp)} + \dot{i}_{out}^{ep} + \dot{i}_{we}^{(cp)} + \dot{i}_{we}^{(ep)} = \sum_{j}^{cp} \dot{M}_{j}^{(out)} \sum_{k} X_{kj} \psi_{k} + \sum_{j}^{ep-g} \dot{M}_{j}^{(out)} \sum_{k} X_{kj} \psi_{k}$$
(1)

$$\hat{i}_{out}^{(t)} = \frac{i_{out}^{(cp)} + i_{out}^{ep} + i_{we}^{(cp)} + i_{we}^{(ep)}}{\sum_{v} P_{P}} = \frac{\sum_{j}^{cp} \dot{M}_{j}^{(out)} \sum_{k} X_{kj} \psi_{k} + \sum_{j}^{ep-g} \dot{M}_{j}^{(out)} \sum_{k} X_{kj} \psi_{k}}{\sum_{v} P_{P}}$$
(2)

$$\dot{i}_{gen}^{(t)} = \dot{i}_{out}^{(cp)} - \dot{i}_{in}^{(cp)} + \dot{i}_{out}^{(ep)} - \dot{i}_{in}^{(ep)} + \dot{i}_{we}^{(cp)} + \dot{i}_{we}^{(cp)} + \dot{i}_{we}^{ep} = \sum_{j}^{cp} \dot{M}_{j}^{(out)} \sum_{k} X_{kj} \psi_{k} - \sum_{j}^{cp} \dot{M}_{j}^{(in)} \sum_{k} X_{kj} \psi_{k} + \sum_{j}^{ep-g} \dot{M}_{j}^{(out)} \sum_{k} X_{kj} \psi_{k}$$
(3)

$$\hat{i}_{out}^{(t)} = \frac{i_{out}^{(cp)} + i_{out}^{ep} + i_{we}^{(cp)} + i_{we}^{(ep)}}{\sum_{P} P_{P}} = \frac{\sum_{j}^{cp} \dot{M}_{j}^{(out)} \sum_{k} X_{kj} \psi_{k} + \sum_{j}^{ep-g} \dot{M}_{j}^{(out)} \sum_{k} X_{kj} \psi_{k}}{\sum_{P} P_{P}}$$
(4)

where $i^{(cp)}_{out}$ and $i^{(cp)}_{in}$ are the rate of PEIs out and in of the system due to chemical interactions within the system respectively, i^{ep}_{out} and i^{ep}_{in} are the rate of PEI out and into the system due to energy generation processes within the system, i^{ep}_{we} and i^{cp}_{we} are the PEI out of a system as a result of the release of waste energy due to energy generation and chemical processes within the system, $M_j^{(in)}$ and $M_j^{(out)}$ are the input and output mass flow rate of stream j, X_k is the mass fraction of a component k in the stream j, Ψ_k is the overall Potential Environmental Impact of chemical k and P_p is the mass flowrate of product p (Okoro et al, 2018).

For the development of the environmental evaluation of the process of bioethanol production from palm rachis, a base case was selected without taking into account neither the energy sources nor the product stream (case 1), and 3 cases where was considered the product stream (case 2), the impacts from energy using (case 3) and the impacts of the flow of energy and products (case 4). The combination of global impact analysis, impacts by category and effect of energy flow and source of energy, allowed to obtain a good diagnosis of the environmental viability of the process.

3. Results and discussion

3.1 Total Potential Environmental Impact (PEI): generated and output

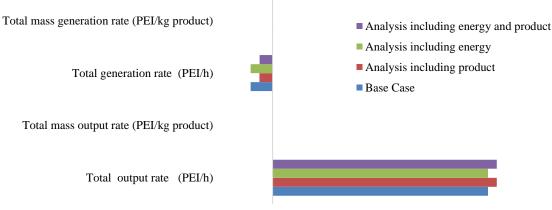
Figure 2 shows the results corresponding to the total PEI generated and total PEI output for all cases. It can be observed that the total PEI generated for each case were negative (-2.25 x 10^3 , -1.34 x 10^3 , -2.25 x 10^3 , -1.33 x 10^3 PEI/h) respectively, which indicates that the process is friendly to the environment ambient. Regarding total PEI output it can observed that for the base case and the case in which the energy is included (case 3) the PEI output values are equal, which indicates that the inclusion of the energy does not generate impacts, while the inclusion of the products generates little impacts.

3.2 Local toxicological impacts of the process: generated and output

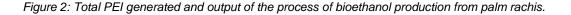
Figure 3 shows the local toxicological impacts generated and output of the process, which includes humans (HTPI and HTPE) and ecological (ATP and TTP) impacts. It can be evidenced that the output impacts directed on humans are more significant compared to the ecological output impacts for all 4 cases studied. In addition, output TTP and HTPI value is the same (5.88 x 10³ PEI/h) for cases 1 and 3, and slightly lower than presented for cases 2 and 4 (5.95 x 10³ PEI/h). Regarding the ATP impact category, the PEI output values are considerably small (3.52 x 10³ PEI/h) for the four cases analysed, this indicates that the impacts generated by this process

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on aquatic systems as well as the mass flow which is ejected into the atmosphere are low. Furthermore, the PEI generated in the 4 impact categories, there is a minimum value which suggests that the process have in the product streams less toxic chemical substances with tolerance values limits (TVL) lower than those fed into the system.



-5.00E+03 0.00E+00 5.00E+03 1.00E+04 1.50E+04 2.00E+04 2.50E+04



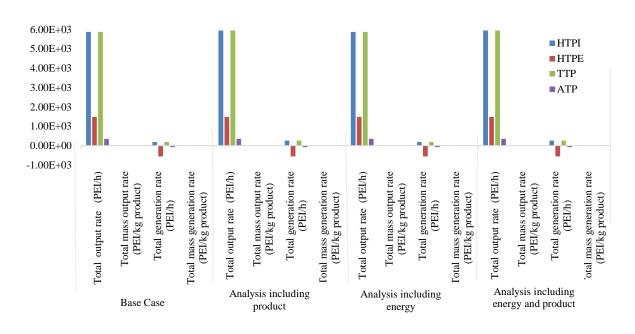


Figure 3: Local output and generated toxicological impacts of the process of bioethanol production from palm rachis.

3.3 Atmospheric impacts of the process: generated and output

Figure 4 shows the atmospheric impacts global (GWP and ODP) and regional (PCOP and AP). It can be observed that values of GWP and ODP are zero in all cases, which leads to the conclusion that the process is neutral under these categories and the use of fuels as an energy source does not contribute to the production of PEI in these categories. The PEI output for AP are (8.39 x 10^3 PEI/h) for all case which is attributed to the emission of chemical substances that contribute to the generation of acid rain, while the PEI output for PCOP category (2.32 x 10 PEI/h) for cases 1 and 3 and (8 x 10 PEI/h) for the other two cases, it can observed that for the last two, the value is slightly higher which is attributed to the inclusion of the product stream.

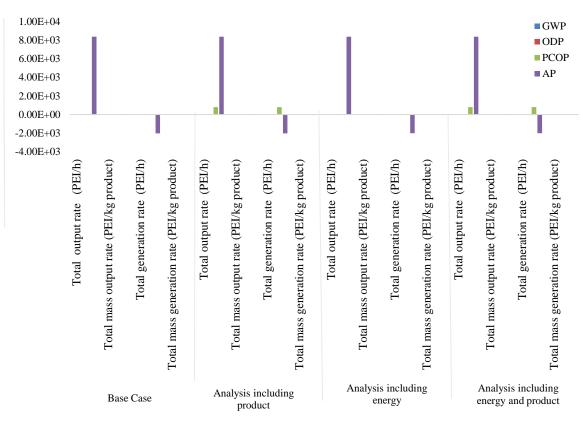


Figure 4: Output and generated atmospheric impacts of the process of bioethanol production from palm

3.4 Effect of energy source

Three types of fuel (gas, coal and oil) were analysed for the evaluation of the impact potential for each of the categories, including the energy and excluding the product stream. The figure 5 shows the changes in the PEI output for each category and for the different fuels used in the bioethanol production process from palm rachis. It can be observed initially that the PEI output are low for each category. However, it can be observed that the use of coal increases the impact in each category, especially in the AP category (2.41 x 10) as well as the ATP category (1.07). Additionally, it can be evidenced that gas as a fuel of the process generates the smallest impacts in each category.

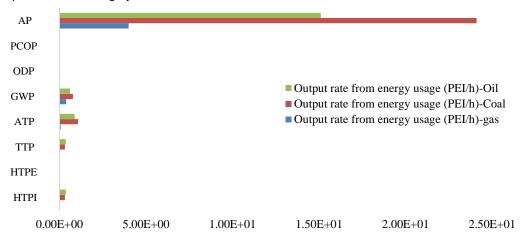


Figure 5: Effect of energy source on output rate from energy usage of the process of bioethanol production from palm

4. Conclusions

The waste reduction algorithm (WAR) was implemented for the environmental assessment of the bioethanol production process from palm rachis. From results obtained it can be said that the process is not harmful to the environment, on the contrary it transforms the feed streams of high PEI into final products of lower PEI, which is reflected in the total PEI generated that are negative values in all cases. in addition, it was obtained that the energy does not generate considerable negative impacts.

Of the total potential impacts generated and output can say with respect to the first that for each case the results were negative, indicating that it is a friendly process from the point of view of potential impacts generated by the process; while the IEP of output for each of the cases does not vary significantly with respect to the base case. On the other hand, from the toxicological impacts it can be evidenced that the exit impacts directed to humans are more significant in comparison with the exit impacts directed to the ecological part in each of the 4 cases studied. In addition, the process has product flows with substances less toxic than those fed into the process, which represents a positive aspect for it; and the impacts to the aquatic environment are considerably small $(3.52 \times 10^3 \text{ PEI/h})$. Finally, with respect to atmospheric impacts, it can be said that the PEI values generated in these categories are low. The PEI output for GWP (1.93 x 10 PEI/h) and AP (1.60 x 10² PEI/h) impact categories in cases 3 and 4, indicates that this process emits chemicals that persist longer in the environment due to their low oxidation and it can also contribute to the generation of acid rain.

Therefore, in general terms, it is valid to affirm that the process as it is designed and with its particularities is environmentally friendly with the environment according to the indications of the WARGUI program used for this study.

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