Multi-objective optimization of an industrial ethanol distillation system using direct and indirect heating

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Abstract
In this work, the performance of an ethanol from sugarcane autonomous distillery simulated on AspenHysys is evaluated using an automated tool programmed on Matlab to assess the environmental and economic impacts associated. We compare the current plant operation (direct heating), located in the South of Brazil, with the use of indirect heating, analyzing vinasse discharge using trucks, as well as the effect of its application in the soil. Results show that the replacement of direct steam injection by reboiler decreases approximately 15% of the vinasse quantity, consequently, decreasing the associated problems generated. Moreover, as the modifications do not change flegma and ethanol flowrates, the revamping might be done without further operational changes. The environmental evaluation presents positive results, showing that the distillery may decrease the eighteen environmental impacts categories assessed. From an economic perspective, the plant could also have higher net profits with the use of reboiler than direct steam injection to heat the distillation column. Finally, the new improved system is treated as a multi-objective optimization problem and it is solved by using the weighted sum method for the Pareto frontier technique to find the best compromise, to be as interesting economically as ecologically.

Keywords: Simulation, Sugarcane vinasse, Economic evaluation, Environmental assessment, Multi-objective optimization.

1. Introduction

Sugarcane biofuel processing has been one of the most important and strategic sectors in the Brazilian economy during the last decades. This sector has steadily increased its activity, propelling all sugarcane-related activities. The Brazilian production of ethanol consolidated in 30.5 billion liters for the 2015/2016 crop, an increase of 6.3% compared to 2014/2015 crop (CONAB, 2016). However, the success of Brazilian distilleries depends on how they overcome the new scientific challenges faced. The traditional sugarcane industry still presents a huge field to be explored, mainly regarding the optimization of process, energy integration, cogeneration, and sustainability (Amorim et al., 2011).

One of the main challenges is related to the reduction of the sugarcane vinasse. This liquid wastewater of the biomass distillation is rich in minerals and is commonly used to irrigate sugarcane crop, known as fertirrigation; however, if produced in excess, it may bring environmental and economic problems. The direct application of vinasse in the soil may cause salinization, leaching of metals present in the soil to groundwater (it also might kill animals and aquatic plants), changes in soil quality due to unbalance of nutrients (mainly manganese), alkalinity reduction, crop losses, increase of phytotoxicity and unpleasant odor (Navarro et al., 2000; Santana and Machado, 2008). Moreover, vinasse is an additional source of greenhouse gas emission to the atmosphere, especially N_2O. Emissions result from aerobic and anaerobic decomposition of the organic matter contained in vinasse that occurs during transportation, temporary storage or after the application in the soil (Oliveira et al., 2013). In Brazil, fertirrigation frequently becomes an economic problem when the area to apply vinasse in the appropriate dosage is not available. This might happen when the crop belongs to the suppliers or it is located far away from the industrial plant. Besides, Brazilian environmental legislation recently established criteria and procedures for vinasse application in the soil. Such environmental technical standard P4.231 (CETESB, 2006) defines the maximum dosage of vinasse to be used in the fertirrigation, which causes problems of surplus vinasse for storage in open lagoons, worsening the aforementioned problems.

Although vinasse use is a topic widely investigated in literature, most of the researches focuses on energy production, treatment before disposal, and yeast production (España-Gamboa et al., 2011; Christofoleti et al., 2013;) and do not study the possibilities to reduce the quantity of vinasse produced. To achieve this objective, the most promising options are concentration by evaporation and the use of indirect heating. Concentration by evaporation reduces the volume of vinasse considerably and it can be used as by-product for animal feed, fertilizer, and fuel for special boilers (depending on the level of concentration); nevertheless, the high-energy demand, fast incrustation of evaporators, and spontaneous crystallization are important limitations of this alternative (Gomes et al., 2011). Thus, replacing direct steam injection by the use of reboiler in the distillation to decrease the quantity of vinasse appears as an interesting alternative to minimize its environmental impacts and economic aspects.

The objective of this study is simulate, analyze, and compare a full-scale industrial system of an alcohol distillery operating with direct and indirect heating using Aspen Hysys process simulator. The models mimic the distillery of the *Cooperativa Agrícola de Astorga Ltda* (COCAFE), which is located in the Northwest of Parana State, (South of Brazil), processing around 180 t/h of sugarcane juice and producing approximately 380 m³/day of hydrated ethanol. No prior work reported in the open literature took into account the use of reboilers in order to decrease the quantity of vinasse produced, analyzing its environmental and economic advantages for distilleries and sugar mills in Brazil. Additional contributions of the present work include: (i) the validation of the simulation results against operational data collected of the industrial plant; (ii) adequacy of the fertirrigation process to the recent environmental technical standard; (iii) the application of an automated evaluation tool to perform a rapid comparison between the scenarios and identify which one is the best alternative regarding both economic and environmental perspective; (iv) multi-objective optimization of the industrial distillation unit, providing the optimum points for the different cost/environmental impacts.

2. Problem statement

In this work, we compare the use of reboiler (UR) to the direct steam injection (DSI) to exchange heat in the first distillation column of the COCAFE distillery. The description of the COCAFE plant, as well as the simulations assumptions can be found in Silva et al. (2015). After the distillation process, which is the first process inside the system boundary analyzed (see Fig. 2), the pumping station sends the storage vinasse to the trucks, which is transported at relatively long distance and then applied in the soil, by broadcaster. The characteristics of this transportation to perform the economic and environmental analysis are: truck capacity of 60 m³, round trip distance to carry vinasse of 90 km, vinasse dosage of 150 $m^3 \cdot ha^{-1}$, and cost per ton $ 0.75 (Zorzenoni et al., 2014; Santos et al., 2015).

The UR and the DSI alternatives are analyzed using two criteria to accomplish a fair comparison between them. Firstly, the simulation is developed on Aspen Hysys 8.6 in order to compare the production of ethanol, flegma (intermediate stream between the first and second distillation column), and vinasse. Secondly, the information in the simulator is used to perform the economic and environmental evaluation programmed in Matlab R2016a. The synergic effects of using both tools simultaneously are essential to improve the performance of the process.

It is important to highlight that as the rest of the activities (evaporation and fermentation systems) is common for DSI and UR, all the economic and environmental evaluations are executed only within the boundary system, which covers the distillation and fertirrigation processes.

2.1 Comparative study of the process alternatives

A comparative study is made setting the mass flow of the stream V1-A to zero $kg{\cdot}h^{-1}$ and removing the adjust block ADJ-1 (see Fig. 2). Furthermore, the variation of vinasse, flegma, and ethanol mass flow is calculated when the direct heating is replaced by indirect heating.

The environmental and economic evaluation of the process alternatives are programmed in Matlab. This tool includes independent modules for the impact assessment based on the material and energy balance and the equipment inventory retrieved from Aspen Hysys simulation used to obtain a rigorous model of the plant. The approach uses a dynamic link using the component object module (COM) technology to connect and send the results to Matlab. Normally, the starting point is a simulation of a configuration with conditions taken from industrial data. Materials, water, and energy consumption per kilogram of product and all other cost indicators are calculated for each configuration. Releases of CO_2 to air, water, and steam consumption are accounted, including electricity and transport for vinasse disposal. Fig. 1 summarizes the procedure followed. Detailed information can be found in Torres et al. (2011).

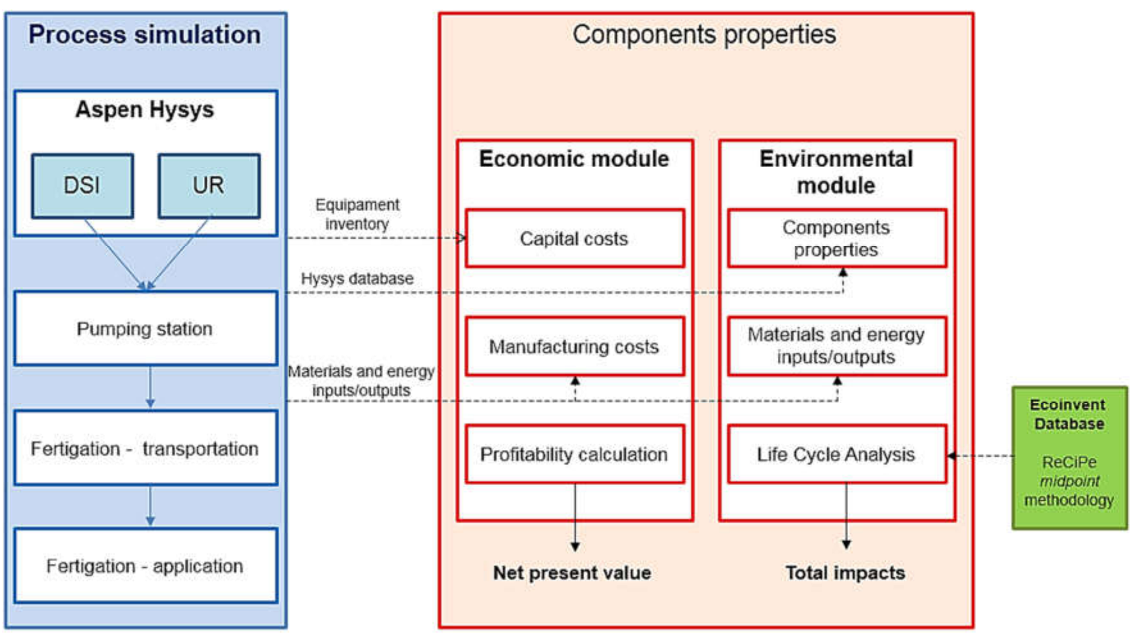

Fig. 1. Flow diagram of the automated procedure for the environmental and economic evaluation based on process modeling.

3. Mathematical formulation

In mathematical terms, the synthesis of chemical processes can be treated as a multi-objective optimization of mixed integer nonlinear programming (moMINLP) problem that accounts for the simultaneous minimization of the total annualized cost (TAC) and environmental impact (EI). In this paper, we apply a systematic methodology for design and optimization of chemical processes that relies on the combined use of simulation and optimization techniques. More precisely, the design task is solved by a simulation-optimization method presented by Brunet et al. (2012) that exploits the complementary strengths of optimization tools (i.e., nonlinear programming, NLP) and commercial process simulators (i.e., Aspen Hysys). The multi-objective optimization methodology is performed only for the configuration that presented the best results for the process after the comparative study.

An external NLP solver in Matlab is employed for searching the values of the design and operating variables that minimizes the total cost and the environmental impacts of the process. As NLP solver, we use the "fminsearchbnd" function that combines "fminsearch" and "fminbnd" well adapted for an objective function type "smooth nonlinear" with constraints. The termination criterion applied is defined according to the upper and lower bounds of each variable (i.e., the algorithm stops when the vectors of upper and lower bounds for all variables are evaluated). Since Matlab function "fminsearch" minimizes a given objective function, we must change the objective function to pose the problem as a moMINLP one. To accomplish this task, it is necessary to obtain gradient information with respect to the objective function and constraints, presented hereafter.

3.1 *Economic objective function: total annualized cost*

The total annualized cost (TAC) accounts for the annual capital cost (CF) and operating costs (CO).

$$TAC = CF + CO \tag{1}$$

The CF represents the cost to purchase and install the reboiler on the column (CR). The Guthries's correlation for economic assessment is adopted for carbon steel kettle reboilers up to 1000 m² of area (Turton et al., 2012) using the most recent Chemical Engineering Plant Cost Index (Chemical Engineering, 2016).

$$C_R = C_p^0 . F_{bm} . F_p \tag{2}$$

where C_p^0 is the purchased cost of the kettle reboiler for the required area, F_{bm} is the bare module factor and F_p is the pressure variation factor according to Turton et al. (2012) and calculated according to Eq. 3:

$$\log_{10} C_p^0 = K_1 + K_2 . \log_{10}(A_r) + K_3 . [\log_{10}(A_r)]^2 \tag{3}$$

The area of the reboiler (A_r) is calculated from the logarithmic mean temperature difference (ΔT_{lm}), the overall heat transfer coefficient (U_r), and the heat duty (Q_r) as follows:

$$A_r = \left(\frac{Q_r}{U_r . \Delta T_{lm}}\right) \tag{4}$$

Finally, the equipment cost is multiplied by the capital recovery factor (crf), which is a function of the interest rate (i) and the plant life cycle (parameter t), which is 20 years.

$$CF = C_R . crf \tag{5}$$

$$crf = \left(\frac{i(1+i)^t}{(1+i)^t - 1}\right) \tag{6}$$

The operating costs are calculated according to direct costs (c_E, c_{SP}, c_{CW}, c_{RM} and c_{WM}) to obtain a final manufacturing cost without depreciation. Then, aiming to optimize the best configuration, the considered factors are electricity demand (E), steam production (SP), cooling water energy (CW), raw materials (RM), waste management (WM) and general operating costs (c_o). For the economic optimization, the total operating cost is thus the sum of all factors.

$$CO = \sum_{m \in M} (E_m . c_E + SP_m . c_{SP} + CW_m . c_{CW} + RM_m . c_{RM} + WM_m . c_{WM} + c_o). top \qquad (7)$$

The operational costs for each equipment unit *m* are calculated by multiplying each factor by its respective price ($/unit) and then by the total annual operating time (top) as shown in Eq. 7. The parameters c_E, c_{SP}, c_{CW}, c_{RM}, c_{WM} and c_o ($/unity) are the unit costs for electricity, steam production, cooling water, raw materials, waste management, and general operations, respectively.

3.2 Environmental objective function and assumptions

The LCIA phase translates the life cycle inventory (LCI) data into the corresponding environmental impacts. The damage in a given category (DAM_d) is determined from the life cycle inventory entries (LCIb) and the corresponding set of damage factors (df_{bd}) as illustrated in Eq. 8.

$$DMA_d = df_{bd} . LCI_b \quad \forall d \in D \qquad (8)$$

In the calculation, all impacts have a coefficient called damage factor that help us to cluster different impact with different units and relative importance into a single indicator (e.g., CO_2 equivalent mass flow for the climate change). In this work, the optimization is performed in terms of climate change (one of the midpoint impact categories present in the ReCiPe methodology), similar to the work of Zhang et al. (2014). Climate change causes a number of environmental mechanisms that affect both the endpoint human health and ecosystem health. The focus of ReCiPe methodology is on the marginal effect of adding a relatively small amount of CO_2 or other greenhouse gases, and not the impact of all emissions (Goedkoop et al., 2009).

4. Solution procedure

One of the main advantages of the approach adopted is that it has benefits from the unit operation models already implemented in the process simulator, which avoids having to define them in an explicit form and the associated physical properties. This procedure facilitates largely the work implemented as it allows optimizing chemical process models already provided by the simulator without having to define the aforementioned equations in an explicit way. To solve the moMINLP problem, the design variables are fixed to the optimal value obtained in the latest iteration of the algorithm. The original problem is first solved by optimizing each single scalar objective separately. In this work, we use the weighted sum method to obtain the Pareto frontier. A key issue in the algorithm is that the process simulator must converge at each time the solver sends a set of values of the design variables. Otherwise, the overall procedure will fail and the solver must automatically go to the next iteration. To ensure this, the NLP is modified to disregard infeasible solutions by adding slack variables and an exact penalty to the objective function. Thus, the modified NLP takes the following form:

$$
\begin{aligned}
(M) \ \min_{x_D} \quad & z = \alpha . f_1(x, u, x_D) + \beta . f_2(x, u, x_D) + \prod (s_1 + s_2 + s_3) \\
s.t. \quad & \alpha = 1 - \beta \\
& h_I(x, u, x_D) = 0 \\
& h_E(x, u, x_D) + s_1 - s_2 = 0 \\
& g_E(x, u, x_D) \leq s_3 \\
& s_1 \geq 0; \ s_2 \geq 0; \ s_3 \geq 0
\end{aligned}
\qquad (9)
$$

In model (M), f_1 is the economic objective function, f_2 denotes the LCA metrics, whereas $\prod$ is a penalty parameter vector, and s_1, s_2, and s_3 are vectors of positive slack variables. As observed, α is the economic cost weight and β is the environmental impact weight. Both, α and β vary from zero to one, thus giving rise to different results to obtain a Pareto curve where all values are optimal. Functions h_I are implicit equations solved by the process simulator (e.g., mass balances), whereas h_E and g_E are explicit external equality and inequality constraints (i.e., temperature of fermenter and vinasse to storage, ethanol composition, ethanol volume flow). The continuous design variables are given by x_D, whereas x denotes the remaining process variables calculated by the simulator, and u represents fixed parameters not modified during the calculations. Note that x_D includes only continuous variables (e.g., heat flow, pressures, temperatures, flow rates). The task to decide among the different alternatives is performed by the decision maker, according to their preferences.

A termination criterion that works well in practice is to stop when the pre-defined number of Pareto points is generated. One of the main advantages of this approach is that it ensures that the solution found is at least locally optimally, as opposed to other meta-heuristic approaches that do not present this property (Brunet et al., 2012).

5. Results and disussions

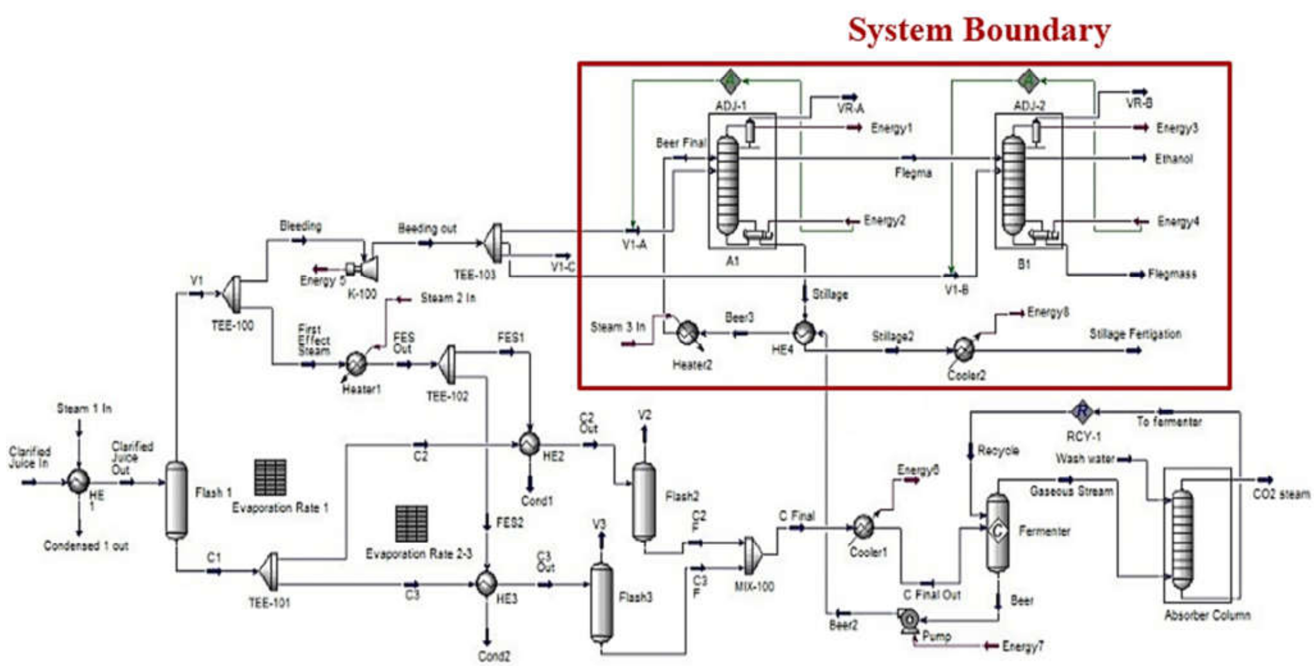

Fig. 2. COCAFE industrial Hysys model operating with direct steam injection.

5.1 Comparative study

There is a significant decrease (15.84%) of the vinasse produced by performing the replacement of DSI by UR. Decreasing the amount of this by-product means that the environmental and economic problems associated are also minimized. In addition, the production of flegma has a marginal variation and the ethanol remains constant (achieving the desired composition), which is assured by the specifications of the distillation columns during the simulation step. This study shows that at industrial level the replacement proposed can be implemented without any effect on the productivity. Moreover, there is a reduction of 24.31% in the amount of energy used to cool the vinasse before storage and a lower energy consumption by the reboiler (around 83%) when compared to the heat flow of the steam used to heat the distillation column in the current configuration. One of the advantages of this new configuration is related to the fact that the steam used in the reboiler returns to the boiler, giving rise to an additional alternative to optimize the heat integration of the process, as well as reducing the operating cost of the plant.

Frame 1 shows that the capital investment costs of the UR are higher than DSI (more than 27%) due to the need of acquisition and installation of the reboiler, which is the main difference between these two configurations. Contrarily, the cost of waste treatment (the most expensive operational cost inside the system boundary) is lower when direct steam injection is replaced by the use of reboiler (7.21% lower) due to the reduction of more than 15% in the vinasse production.

Frame 1. Capital costs and operating costs producing ethanol and fertirrigation process alternatives for direct and indirect heating.

	Direct Steam Injection ($)	Use of Reboiler ($)	Variation (%)
Capital investment costs			
Reboilers	274,749	350,636	27.62
Manufacturing cost (yearly)			
Waste treatment	1,261,237	1,170,296	-7.21
Utilities			
Electricity	151,880	151,880	0
Steam (LP/MP/HP)	158,863	41,050	-74.16
Cooling water	198,915	178,829	-10.10
Operating labor	331,695	331,690	0
Other manufacturing costs[a]	538,631	739,660	37.32
Total	2,641,221	2,613,405	-1.05

[a] It includes maintenance, repairs, operating supplies, local taxes, insurances, plant overhead costs, and administration costs (Turton et al., 2012).

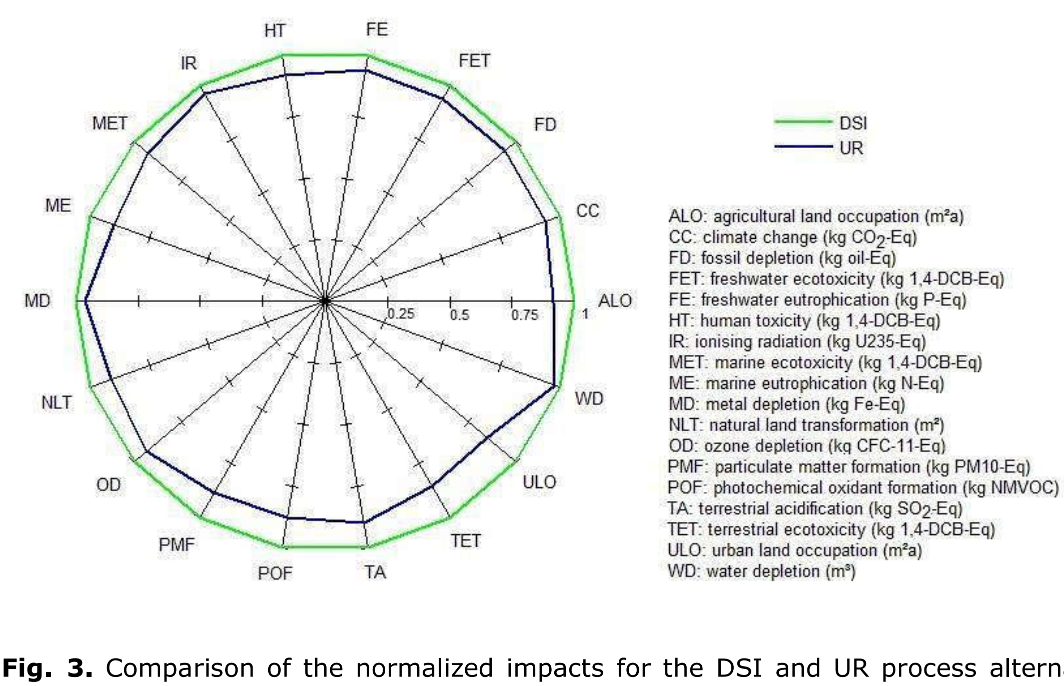

Fig. 3. Comparison of the normalized impacts for the DSI and UR process alternatives following the ReCiPe methodology.

The impacts of each category are calculated following the ReCiPe midpoint impact assessment methodology, considering 1kg of ethanol produced as a functional unit. The values obtained are normalized by the impacts of the current configuration and all of the eighteen category impacts are included (Fig. 3). The UR configuration has lower impacts in all categories when compared to the DSI and the most significant reductions are related to urban land occupation (reduction of 15.05%) and terrestrial ecotoxicity (reduction of 14.73%). Reducing the amount of organic dry matter content and soil loss are some of the increasingly concerns for the agricultural section of the ethanol process. It also supports the industrial plant to attend the specifications present in the environmental technical standard P4.231. The reduction of terrestrial ecotoxicity, regarded to the toxic effects of chemicals on an ecosystem, may avoid biodiversity loss, contributing to build a more sustainable industrial plant.

5.2 The Pareto frontier

The multi-objective optimization is applied to the UR configuration, which presented the best results for both economic and environmental assessment. Its results are in agreement with those expected. All points are Pareto frontiers, but during the optimization, many suboptimal points were obtained and those that were dominated were removed from the analysis. This occurs in non-linear problems when the solver is trapped in a local minimum or maximum, which is a common problem in complex models.

Two different parts are identified in the Pareto curve (Fig. 4). On the first part, from the left to the right, the impact is decreased by using less electricity and slightly increasing the flegmass (bottom product of the second distillation column) and vinasse volume flows. It leads to a reduction of the environmental impact by comparison with the cost decrease (1.73% reduction). On the second part, the flegmass and vinasse volume flows are virtually identical for all configurations. More electricity power and more cooling water are used to compensate the temperature and pressure modifications concerning the clarified juice and the wash water used in the absorber column. The result is a low impact decrease compared to a high cost increase (8.29% variation). In fact, in this case we take into account the CO_2 stream leaving the process.

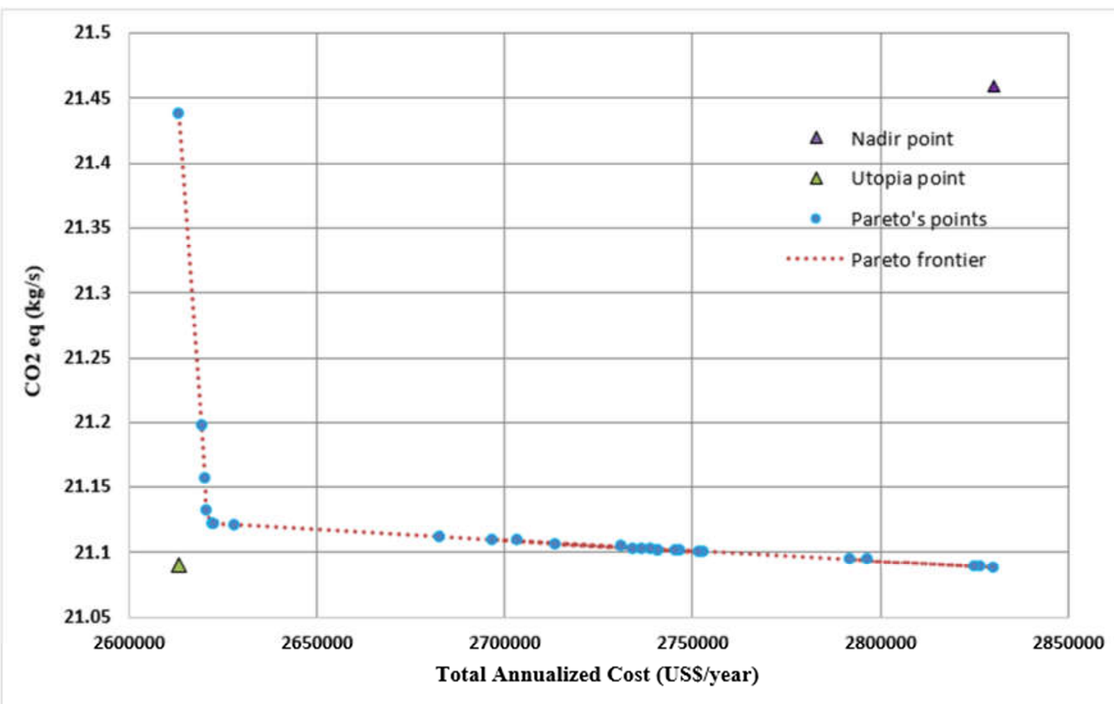

Fig. 4. Pareto set of solutions for the climate change versus TAC.

From Fig. 4, it seems that the most interesting operation point for climate change is around the so-called "knee point", which is located at the intersection of the two sections of the Pareto frontier. That is, the optimum is the nearest point to the utopia point, which represents the optimum cost and optimum environmental impact (impossible to reach). The set of individual optimums $f^U = [f_1^*(x_1^*); f_2^*(x_2^*)] = [2{,}613{,}411; 21.09]$ represents the utopic point, while the set of maximum values (non-optimums) $f^N = [f_1^N(x_1^N); f_2^N(x_2^N)] = [2{,}830{,}242; 21.44]$ indicates the Nadir point. Overall, it is possible to evidence the improvement of the plant including reboiler once the current plant operation point is distant from the Nadir point of the proposed scenario, making it unfeasible to show both points on the same graph for the multi-objective optimization.

6. Conclusions

This work demonstrates that a validated process simulation automatically integrated to a mathematical programming is a powerful tool to evaluate the performance of a wide range of industrial processes. It can help us to find the best configuration among a set of alternatives, as well as the viability of revamping projects.

The adapted evaporation process was successfully integrated into the distillation process, inserting the fermentation and ethanol recovery process in Aspen Hysys 8.6. The comparative study between direct steam injection and the use of reboilers in the distillation process showed a reduction of 15.84% in the quantity of vinasse produced with a marginal effect in ethanol and flegma products. In this way, the environmental and economic impacts caused by vinasse are minimized, while the quality and productivity of the plant is maintained, adjusting the plant to the recent environmental technical standard.

Replacing direct by indirect heating, the economic assessment presents a high profitability with a positive NPV of the project of U$77,184. This high profitability is mainly due to reduction of the vinasse quantity. Furthermore, the environmental evaluation revealed that all the impacts of the proposed configuration (use of reboiler) are lower when compared to the direct steam injection. In this scenario, the categories terrestrial ecotoxicity and urban land occupation represent the most significant reductions (more than 14%).

For the improved scenario purposed, we optimized an operational ethanol distillation system using an external optimizer (Matlab) considering simultaneously the cost and the environmental impact. The profile of the curves indicates that the environmental impact can be further reduced with a marginal effect in the cost.

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