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A Screening Design to Analyze the Influence of Technological Configurations on Techno-economic Parameters for Autonomous Distilleries in Brazil

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This study aims to assess how Internal Rate of Return of the enterprise, Ethanol Output and Surplus Electricity vary according to changes in existing scenarios of an autonomous distillery, that is, a distillery producing ethanol and electricity, but not sugar. A simulation procedure using the Virtual Sugarcane Biorefinery (VSB) framework according to a screening design is used for this purpose. The VSB is composed of a set of computer-aided tools to simulate the sugarcane agricultural production system, its transport as well as the industrial processing. The sensitivity of operational variables, such as fermentation yield, steam consumption, boiler steam pressure, juice extraction yield, residual ethanol concentration in vinasse and alcohol content in wine were varied in a realistic basis, constrained by operational limits, which resulted in forty-five scenarios following a Central Composite Design (CCD). This design was used to describe ethanol production possible scenarios in autonomous distilleries in Brazil. This procedure has allowed evaluating scenarios with different technological configurations. The influence of these operational variables on the techno-economic parameters was studied through a screening procedure for statistical evaluation of results.

1. Introduction

Mathematical models have been widely used as decision support tools for the analysis of complex problems in industrial environments. A well-adjusted model is capable to predict the process behavior and provides a way to evaluate the impacts of the process parameters and operational conditions on techno-economic parameters, which comes to be a practical and inexpensive way to obtain information about the system.

In order to highlight the most important parameters for a given response under analysis, many simulations have to be run covering a number of alternative scenarios. Thus, it is possible to have a better guideline for assessing the techno-economic attractiveness of best available technological configuration.

In this context, screening methods are presented as a useful tool to quantify the impact of input variations on a given model response (Ruano et al., 2012). Therefore, if a small change in an input variable leads to a large variation in a certain response parameter of the model, this variable is considered important and its determination must be as precise as possible (Cangussu et al., 2003). Assuming that only some input variables contribute significantly to the outcome, screening methods facilitate the data collection by limiting the maximum precision to inputs considered the most important (Rivera et al., 2013). Besides being used to obtain information about the degree of importance of each variable, screening methods are frequently used to validate the model itself. This validation indicates whether or not the model follows an expected behavior.

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Screening procedure can be performed through Design of Experiments (DOE) techniques, in which the aim is to investigate which of the operational variables are the most influential for each techno-economic response obtaining, therefore, optimal value for each operational variable. This suggests that, before the fitting procedure, it is required to select the points within the input variables domain where experiments are conducted. Thus, in this study, a Central Composite Design (CCD) (Montgomery, 2001) was selected to represent the domain of interest of the operational variables in a Brazilian autonomous distillery to analyze their influence on techno-economic parameters.

The first generation (1G) ethanol production, a denomination for ethanol produced trough the fermentation of sugar cane juice, in an autonomous distillery comprises the following main steps: sugarcane cleaning, extraction of sugars, juice treatment, juice concentration and fermentation (the traditional Melle-Boinot process, i.e. a fed-batch culture where yeast cell is reused from successive fermentation), distillation and dehydration (using molecular sieves). In this process configuration the sugarcane bagasse, a cellulosic agro-industrial by-product, is used as fuel in a cogeneration system to generate steam and electricity (Dias et al., 2013).

The interest in broad aspects of autonomous distilleries is to contribute with social, energy security, economic and environmental aspects (Ensinas et al., 2013), usual motivation for biofuel production. Thus, a current concern is how changes in technological configurations of autonomous distilleries can influence in the system techno-economic analysis.

This study aims assessing how the Internal Rate of Return (IRR), Ethanol Output (EO) and Surplus Electricity (SE) vary according to changes in the existing scenarios of an autonomous distillery. A simulation procedure using the Virtual Sugarcane Biorefinery (VSB) developed at the Brazilian Bioethanol Science and Technology Laboratory (CTBE/CNPEM) based on previous screening design is used for this purpose.

The VSB consists of a set of computer-aided tools, including simulators of industrial processes, spreadsheets and Life Cycle Assessment software. A spreadsheet named CanaSoft was developed to simulate the agricultural stage, which includes all sugarcane agricultural operations from pre-planting to harvesting and transport. Furthermore, many industrial scenarios of biorefineries are assessed through sequential modular simulation with Aspen Plus®. In this sense, the VSB is presented as a tool to assess the techno-economic and environmental impacts of new technologies associated with the productive chain of sugarcane biorefineries.

It is clear that VSB requires many parameters and variables to represent the complexity of the simulated system, however, because not all parameters have the same influence on the VSB outputs, the present study is useful to evaluate whether changes in particular operational variable values in industrial stage leads to large changes in techno-economic parameters.

2. Methods

An effective screening design for sensitivity analysis follows a standard approach, regardless of the scenario and the case study. In general, sensitivity procedures may be summarized as follows:

- Catalog all the input variables of the model under study. It is important to highlight that these inputs present different degrees of importance on both VSB models and the real process.
- Even in a model with many variables, the sensitivity analysis of a certain scenario is performed just with the inputs that are more likely to have a significant impact on the response under study. Therefore, among all the input variables, the key ones were chosen to undertake the analysis.
- With the key inputs, the range of these variables may be defined. In this study, the intervals were established through the definition of usual values. The most representative intervals of current ethanol production processes in Brazil are termed usual values. Therefore, this analysis involved the collaboration of specialists in the sugarcane sector and the CTBE research team.
- The sensitivity analysis of the studied responses is carried out. In this study, the sensitivity procedure was performed by a Central Composite Design (CCD).
- The sensitivity analysis results are validated. The validation criteria were based on the adequacy that is expected for the actual ethanol production process in Brazil. Again, the collaboration of the CTBE research team was necessary in order to confront the technical knowledge of the actual scenario with the results achieved by the CCD methodology. This gave a more precise and significative overview to the sensitivity analysis performed.

Table 1: Values of the key inputs in Central Composite Design

Input	Description	- α	-1	0	1	+ α	Unit
1	Fermentation yield	88	89.2	90	90.8	92	%
2	Reduction on steam consumption	10	15.8	20	24.2	30	%(Steam 2.5 bar)
3	Boiler steam pressure	21	43.9	60.5	77.1	100	bar
4	Juice extraction yield	93	94.3	95.3	96.2	97.5	%
5	Residual ethanol concentration in vinasse	100	186.9	250	313.1	400	ppm
6	Alcohol content in wine	7	8.2	9	9.8	11	°GL

In this study, six key inputs were chosen, namely operational variables: Fermentation Yield (FY), Reduction on Steam Consumption (RSC), Boiler Steam Pressure (BSP), Juice Extraction Yield (JEY), Residual Ethanol Concentration in Vinasse (RECV) and Alcohol Content in Wine (ACW).

The influence of these operational variables on the Ethanol Output (EO), Surplus Electricity (SE) and Internal Rate of Return (IRR) has been studied with the sensitivity analysis performed by a CCD. EO and SE were obtained directly from simulations of 1G ethanol production in an autonomous distillery model developed using the Aspen Plus® (version 7.3.2, Aspen Technologies, Cambridge, MA) in VSB framework. Economic data suitable to the Brazilian situation were collected and an electronic spreadsheet with Visual Basic macros was developed to calculate IRR. Details of the economic analysis are described elsewhere (Dias et al., 2011).

In CCD, the inputs assume five different values inside the intervals. The axial values (± α) in this study are the upper and lower boundaries of the intervals defined as the most representative of the current ethanol production process in Brazil. The central values (0) and the intermediates (-1 and +1) were calculated through a proportionality rule. Table 1 summarizes the key inputs in CCD.

The CCD matrix is composed by thirty-two half fraction factorial points (2^{6-1} of resolution V), twelve axial points and one center point. Thus, forty-five simulations of 1G ethanol production were performed for the CCD in an autonomous distillery model developed in Aspen Plus®. Statistical analysis of the data obtained in the design was carried out using the software Statistica (version 12, Statsoft Inc., Tulsa, OK). In this analysis, Pareto charts have provided the magnitude of the effects of the input variables on the responses studied. The effect estimates divided by their standard errors are sorted from the largest absolute value to the smallest absolute value. The magnitude of each effect is represented by a column, and a line going across the columns indicates how large an effect must be to be considered statistically significant. In this study the vertical line corresponds to a p-value of 0.01, which implies a 99% level of significance.

3. Results and Discussion

Sensitivity analyses were performed and the inputs were ranked in order of importance. The magnitude of the main effects and their interactions can be observed in the Pareto charts shown in Figures 1 to 3. It can be seen from these charts that only some main linear effects for responses under study (EO, SE, and IRR) are statistically significant at 99%. The linear and quadratic effects are denoted by the indices (L) and (Q).The statistically important inputs for each response are summarized in Table 2.

The proposed screening method coupling DOE and VSB simulations can convert the correlation of the decision operational variables and techno-economic parameters into simplified mathematical models (Equations 1 to 3) and suggesting subsets of the decision operational variables that can be considered in further optimization studies.

$$IRR = 0.139 + 0.00167\, X_1 + 0.00138\, X_2 + 0.00299\, X_3 + 0.00204\, X_4 \quad (1)$$

$$EO = 58.75 + 0.476\, X_1 + 0.524\, X_4 \quad (2)$$

$$SE = 80949248.3 + 1988543.3\, X_2 + 7837216.2\, X_3 \quad (3)$$

In these equations X_1, X_2, X_3, and X_4 are the coded values of FY, RSC, BSP, JEY.

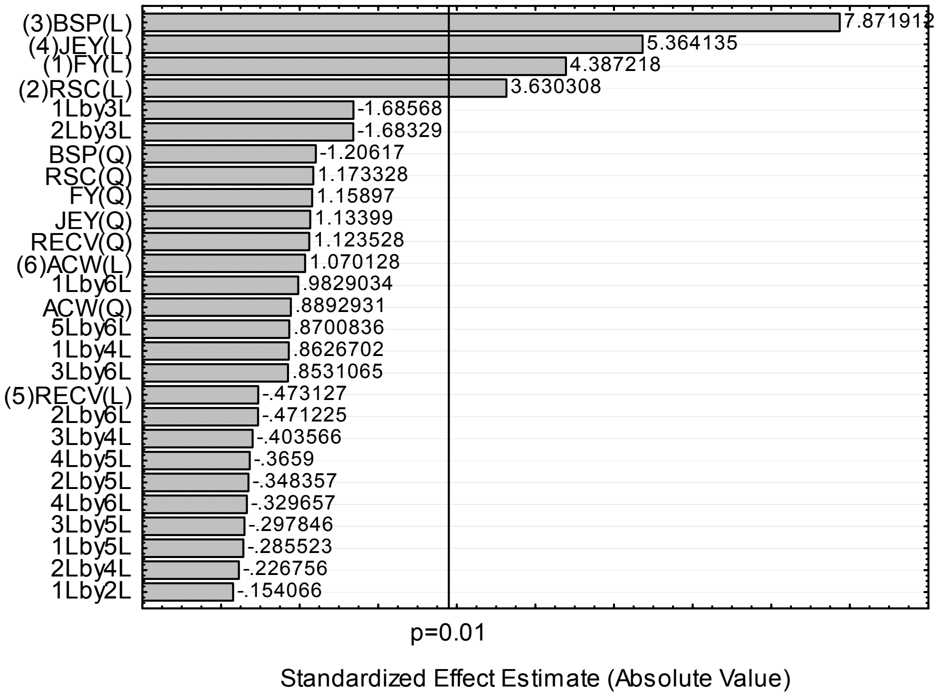

Figure 1: Pareto chart of standardized effects for the response Internal Rate of Return (IRR)

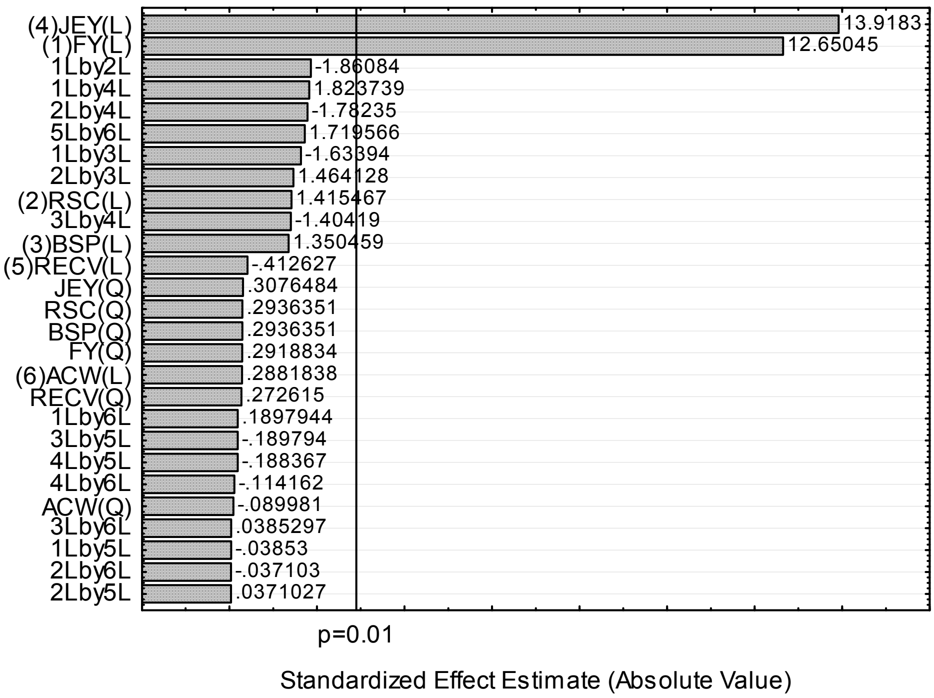

Figure 2: Pareto chart of standardized effects for the response Ethanol Output (EO)

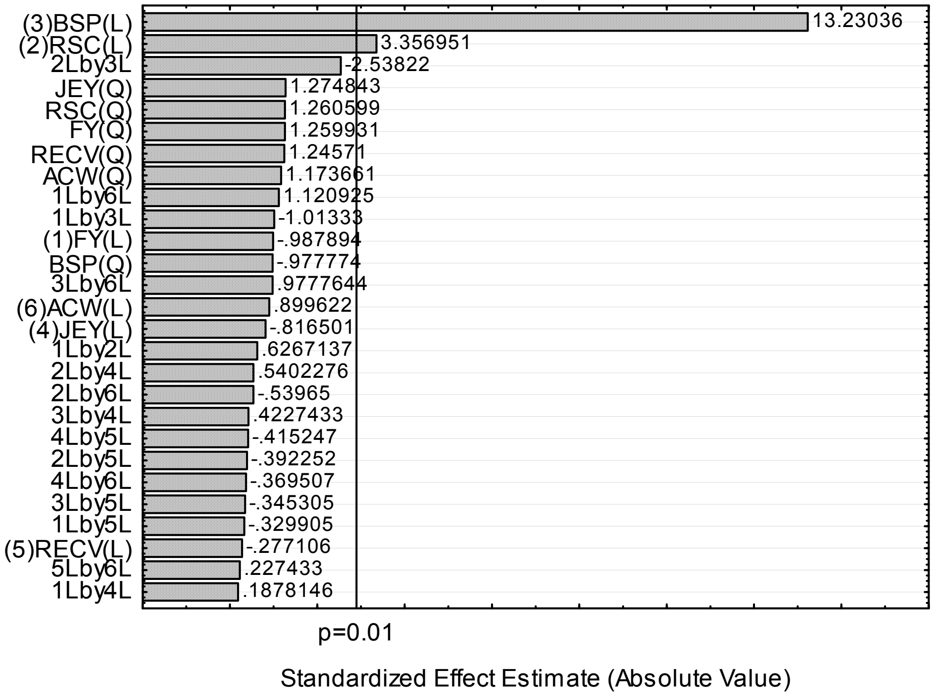

Figure 3: Pareto chart of standardized effects for the response Surplus Electricity (SE)

Table 2: Most statistically significant inputs for each response under study

Input	Description	IRR (%)	Ethanol Output (m^3/h)	Surplus Electricity (W)
1	Fermentation yield	X	X	
2	Reduction on steam consumption	X		X
3	Boiler steam pressure	X		X
4	Juice extraction yield	X	X	
5	Residual ethanol concentration in vinasse			
6	Alcohol content in wine			

Some conclusions that come from the sensitivity analysis are general, regardless of the analyzed response. The results show that the most important inputs affect the responses linearly. Additionally, the positive sign of these effects means that these inputs have a directly proportional relationship with the responses. These two findings improve the knowledge about how changes in the inputs influence the EO, ES and the IRR. They allow a better understanding of the sensitivity results and the comprehension of both Aspen Plus® simulations and the actual ethanol process production. The IRR value is a useful parameter to compare different investment alternatives and assess the economic viability of a project. Comparing two investments, the most attractive will be the one which has the higher IRR.

The boiler steam pressure is directly related to the electricity cogeneration. More electricity will be produced by the plant with a higher boiler pressure. This electricity is used to supply the plant requirements and the surplus is sold to the grid, having a positive impact on the profitability.

Other gain in profitability may be achieved through increasing the yield in juice extraction and in the fermentation step. The juice extraction yield is the efficiency with which sugars available in the sugarcane are recovered in the juice. A higher yield means that a larger amount of sugar will be available to the fermentation process without increasing the amount of milled cane.

In a 1G autonomous distillery, a higher yield in the fermentation reactor leads to a higher ethanol production, since all the extracted juice is sent to this process. At last, decreasing the consumption of steam through energy integration in the plant benefits the profitability because there will be more steam available for electricity production, increasing the fraction sold to the grid. As a conclusion from the previous analyzes, it is justified that these four inputs are statistically significant to the IRR.

The ethanol output is related to the amount of ethanol produced per hour in a 1G autonomous distillery. Increasing this output is one of the major concerns in these distilleries, since this value is directly connected with the plant efficiency and profitability. In the sugarcane industry, the extraction process is of great importance, because all the following steps to obtain ethanol depend on this operation. As mentioned before, the amount of ethanol will increase for the same quantity of milled sugarcane when this yield is increased. The fermentation yield is also important because increasing this value is directly linked with the efficiency to produce ethanol in the fermenter. In face of this analysis, it is justified and expected that these two inputs are statistically significant to the Ethanol Output response.

Surplus Electricity is the excess energy produced by the distillery through the cogeneration process. With a higher surplus, the ethanol plant may increase its profitability by selling electricity to the grid. Both the steam consumption and boiler steam pressure are important to the electricity production. This fact is explained through the same arguments given in the IRR analysis. Thus, it is justified that these inputs are statistically significant to this response.

4. Concluding Remarks

The screening procedure has been successfully used to evaluate the relevant variables to 1G ethanol production in an autonomous distillery. In this procedure, the CCD coupled to VSB simulations was shown as particularly efficient to obtain information about the significance of the operational variables, as well as helping to identify more clearly the structure of the VSB, since the potentially most significant variables are explicitly presented, and the effectiveness of this tool in emulating the productive chain of sugarcane biorefineries is confirmed.

This approach can be applied straightforward to several potential biorefinery configurations (e.g. annexed plants, second generation biorefineries, among others), as well as the complete production chain.

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