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SIMULATION AND OPTIMIZATION FOR A LIGNOCELLULOSIC BIOREFINERY CONSIDERING SOCIAL, ECONOMIC AND ENVIRONMENTAL INDICATORS

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Abstract: This research raises and solve the simulation and later multi-objective optimization problem of a lignocellulosic biorefinery, considering an economic, environmental, and social aspect. The biorefinery produces from the residue corncob, until five biochem- ical products: xylitol, succinic and lactic acid, bioethanol and lignosulfonate. In the simulation of the biorefinery, we choose eleven decision variables based on a previ- ous sensibility analysis for their response in the economic and environmental objective function. The economic and environmental objective function were measured with the economic profit and the global warming potential by the CO_2 emissions. The novelty relapse in the social index, that is formulated based on three social indicators reported by Mexican government and what allows us to identify and propose five possible loca- tions of the biorefinery. Finally, the optimization results will determine which of the five locations, in addition to configuration and production of the biorefinery, were the best.

INTRODUCTION

A biorefinery is a production plant that uses biomass as a raw material to produce: fuels, chemicals or energetics. Any organic, available and renewable substance could be biomass, with the potential to replace fossil fuels and petrochemicals. There are many kinds of biore- fineries, most of them, uses corn and soy as a feedstock. This situation is very questionable because of competing with human consume of those food. That is the reason why it is important to focus on the study of second generation of biofuels, where the lignocellulosic biomass comes from a residue.[1] The lignocellulosic feedstock we selected was corncob, it is a cheap, available, and with specific composition (low protein), that make it unsuitable for animal feed. [2] According to a study by the International Energy Agency, the production of second-generation biofuels in developing countries such as Mexico, is attractive for the search for domestic or international financing, highlighting the fact of evaluating the energy benefits that could have biomass. It is important to take care in the availability of water required by the process, as well as collect reliable and representative data on the economic, environmen- tal and social area, with the objective of create specific conclusions and recommendations to each country.[3]

Sacramento-Rivero et al. make a SWOT analysis (Strengths, Weaknesses, Opportunities, and Threats) of the situation of the biorefineries in Mexico and conclude that the develop- ment of a national industry of biofuels is a necessity more that an option. They insist that in order to achieve an economic feasibility, it is necessary to produce high value bioproducts and not only biofuels. Although the legislation to regulate that actions directed to that objective already exist, because of the wide process options that are, it is important to have a national strategy that establish priorities and a chemical portfolio in order to ease local markets.[4] In our study, the five biochemicals that biorefinery can produce, have a market in our country because we know there are more imports that exports of those items.[5]

Regarding the Process System Engineering area, Garcia and You did a review for Water-Energy-Food-Nexus literature. They noticed the huge opportunity in studding the three aspects simultaneously. The few studies out there sometimes uses life cycle assessment in the optimization model. Also they mentioned real examples of real-world WEFN problems with potential to be studied. They conclude that typically, only two of the three dimension of the WEFN were studied at the same time. Studied the three dimensions at the same time has a lot of challenges and unpredicted consequences. Another important aspect they mentioned is to clearly define the system boundaries.[6]

In a sustainable process, it is necessary to satisfy the next three aspects: environmental, social and economic. There are plenty chemical process indicators for environmental and economic aspects; in fact, exists additional classification that depends on the stage or the process.[7] According to Ruiz-Mercado et al., several social indicators have been proposed in previous studies, the majority representing qualitative or semi-quantitative aspects of industry, such a safety aspects for employees. Most of the social indicators, are based on relative criteria that are not easy to measure or relate to the quantitative data of the process.[7] The Miret et al. study is interesting because they did, like us, a multi objective op- timization considering the economic, environmental and social benefit. They propose a superstructure including all the supply chain regarding the biorefinery including harvesting, storage, pretreatment, conversion and distribution. The social benefit is measured by the generated jobs, not only the direct ones but also indirect and induced jobs. The economic objective function was quantified as the sum of all the operating costs of the supply chain. Finally, the environmental criteria was calculated by an ecocosts method. Ecocosts are a measure that expresses the environmental load of a product on the basis of prevention of that burden during the product life cycle: from the raw materials until its end of life.[8] According to Dowling et al., when solving multi-objective optimization problems, there are two fundamental problems that must be addressed: dimensionality and ambiguity.[9] That is why they proposed a decision-making framework to compute compromise solutions that balance conflicting priorities of multiple stakeholders on multiple objectives. They use a ge- ometric interpretation of a Conditional Value at Risk (CVaR) to prove that any compromise solution obtained with the framework they proposed is a Pareto optimal solution of the origi- nal problem.[9] Similar concern about this topic present Roth et al., they consider what seems to be missing in their opinion is a holistic approach that would gather expert knowledge in social, environment, economy, and engineering areas and that would be generic enough to apply to any development process, including chemical engineering plant installation. The framework they proposed, described and assessed the project with the four views recom- mended by the ISO 19440 standard: architectural, structural, functional and behavioural. [10] The model we present at this work, the framework of the social objective function, has the flexibility of assign different values for the environmental, economic, and societal metrics as we use as indicators. That is important because depends on the stakeholders involved, these values could change.

It is common that some authors approach the environmental objective function in their studies analysing the Life Cycle Assessment (LCA). Gerber et al. compare in their article, the results of a conventional LCA analysis with the obtained from the Life Cycle Impact Assess- ment (LCIA) in a process of synthetic natural gas and electricity production obtained from lignocellulosic production.[11] In this study, the environmental objective function is measured by estimating the CO_2 emissions coming from auxiliary services for heating and cooling, also the emissions from the different stages in the processes. In the Gerber et al. article, the economic function is the sum of the system operating costs, so the objective is to minimize this function. However, in d'Amore and Bezzo study, this objective function is calculated in terms of global Net Present Value so this objective function need to be maximized.[12] Gebreslassie et al. proposed a bi-criteria NLP problem to address the optimal design of sustainable hydrocarbon biorefinery that produce gasoline and diesel from hybrid poplar biomass via fast pyrolysis, hydrotreating and hydrocracking. In the environmental objective function, they also used the LCA and minimized the Global Warming Potential (GWP) and for the economic objective function they maximized the Net Present Value (NPV).[13] In our case, regarding the economic aspect, we calculated this function by the annual profit, so this function also need to be maximized. The study of Gebreslassie et al. is similar of ours because they also did a rigorous model in the simulation of the biorefinery, we also evaluate the economic and the environmental aspect simultaneously, and we also included the social aspect with a novel methodology we explain in forward sections.

Ehrenstein et al. worked and propose a methodology to optimize supply chains threatened by rare event disruptions, for example extreme weather events, in terms of their economic and risk performance, this one evaluated via CVaR and Worst Case(WC). They used the augmented epsilon-constraint method (AUGMECON) and applied their method on two case studies already solved and get the solutions with a time reduction of 99%. [14] In the d'Amore and Bezzo article, they solved a bi-objective considering the economic and environmental performance, they modelling the multi-echellong supply chain.[12] They chosen northern Italy as the case study and discretize according to the grid approach described by Zamboni et al., consisting of 59 square of equal size. [15] In the present study, we discretize all the Mexican territory with the political division, that is because the facility to find information concerning their social indicators for the construction of the social objective function.

Yeh et al. investigates the economic impact of a biorefinery on an established timberlands system, they separate the objective functions in the bilevel problem and compare with the single level, finally they conclude that the bilevel model describe more accurately the real system.[16] Another study of biorefinery involving wood as a feedstock is the Mansoornejad et al., where used mixture of wood chips, forest residues, sawmill residues, and hog fuel. The product of the biorefinery involves succinic acid, malic acid, lactic acid and xylitol as a coproduct.[17] In our study we also produce succinic acid and xylitol as a biorefinery products, but instead of malic acid we also produce ethanol, lactic acid and lignosulfonates. A similarity between the Mansoornejad et al. study and ours is the flexibility of the system but we just simulate and optimize the biorefinery and these authors show the entire study for a supply chain since suppliers until final customers.

There are some studies such the L´opez et al. or the Corbetta et al., that develop a strategy of solution of a multi-objective optimization problem based on some study cases and compare the solution and the convergence time according to the methodology of solution selected. In the first case, Aspen and CasADi have been selected as the tools for computer- aided engineering in order to enable MOO in a flowsheet simulator,[18] while in the second case they use the process simulator PRO/II, and an algorithm implemented in C++ and GAMS.[19] In our study we simulate and optimize with Matlab.

In the following sections, we explain in detail the methodology of the simulation of the biorefinery, the development of the three objective functions we evaluate, with special detail on the proposed social index. Then we present the results of the simulation and later opti- mization, and finally we conclude about the study we present.

MATHEMATICAL BASIC CONCEPTS

The general multi-objective optimization problem is considered as follows:

$$\min_{x} \mathbf{F}(x) = \min_{x} [f_1(x), f_2(x), ..., f_n(x)]^T \quad (MOOP)$$

subject to:

$h_j(x) \; = \; 0, \; j = 1, 2, ..., m$
$g_k(x) \; \le \; 0, \;\; k = 1, 2, ..., p$

where n is the number of objective functions, m is the number of equality constraints, and p is the number of inequality constraints. $x \epsilon R^l$ is a vector of design variables, also called decision variables, where l is the number of independent variables x_i. $\mathbf{F}(x) \; \epsilon \; R^n$ is a vector of objective functions $f_q(x)$. $f_q(x)$ are also called objectives or cost functions. The objective functions are assumed to be conflicting so that one cannot be minimized without increasing the other, this situation gives rise to the concept of a Pareto solution.

Pareto solution is a feasible point x^* for the multiobjective optimization problem (MOOP) is said to be Pareto optimal if and only if there exists no other feasible point (x) such that $f_q \; \le f_q(x^*) \forall q \; \epsilon \; R^n$ and $f_q(x) < f_q(x^*)$ for at least one index $q \; \epsilon \; R^n$. The family of Pareto solutions form the so-called Pareto front, which represents a limiting curve of performance in the objective space.

The utopia point is a point given by the solution x^u_i with coordinates $f_q(x^u_i)$ in the objective space. The coordinates are given by the solution of $minf_q(x)$ subject to $h(x) = 0$, $g(x) \le 0$, $x \; \epsilon \; R^l$ for $q \; \epsilon \; R^n$. The utopia point is unattainable since the objectives are conflicting; however, it can still be used as a reference point. For instance, it is possible to compute the closest point along the Pareto front to the utopia point, also known as the compromise solution.

The compromise solution is a point, x^s with objective $f\,(x^s)$ given by the solution of the minimum distance problem, usually the Euclidean distance as follows:

$$\min_{x} \left\{ \sum_{r \in R^n} \left[f_q(x) - f_q(x_i^u) \right]^2 \right\}^{1/2}$$

However, it is not necessary to restrict closeness to the case of a Euclidean norm.[20] In addition, if different objective functions have different units, the Euclidean norm or a norm of any degree becomes insufficient to represent closeness mathematically. Consequently, the objective functions should be transformed such that they are dimensionless. One of the most common approaches to scale the underlying objective functions, regardless of their original range, is given as follows: $f^{dl}(x) = (f_q(x) - f_i^{min})/(f^{max}_i - f^{min}_i)$, this approach is consistently referred to as normalization. In this case, $f^{dl}_q(x)$ generally has values between zero and one, depending on the accuracy and method with which $f^{max}_i(x)$ and $f^{min}_i(x)$ are determined.

Multiobjective optimization methods. During the past decades, many methods have been proposed to deal with multiobjective optimization problems. Full reviews can be found in the books by Liu[21] and Yann[22] and the references therein. Traditionally, MO problems are solved by scalarization, [21] e.g., by means of a weighted sum of the objectives. Using some characteristic parameters, the original MO problem is transformed into a single objective optimization problem whose solution is expected to be Pareto-optimal. The parameters can either represent the relative importance of the objectives or be a mere mathematical device which is varied systematically to obtain different solutions. However, from a practical point of view, the user is only interested in one final solution. An additional element in comparison to the single objective optimization is that of the decision user, who is responsible for selecting such a solution. In this work we applied the normal boundary intersection (NBI) to solve the associated Non Linear Programming (NLP) problem.

Now, we are going to describe some of these multiobjectives techniques. Firstly, the Weighted Sum Method (WSM), which is a standard technique for generating the Pareto set in multi- criteria optimization problems is to minimize (convex) weighted sums of the different objec- tives for various different settings of the weights. In other words, n weights w_q are chosen such that $w_q \geq 0$, $r = 1, 2, \ldots, n$, and $\Sigma^{n}_{r=1} w_q = 1$ and the following problem is solved: min $\Sigma n_{r=1} w_q f_q(x)$, subject to: $h_j(x) = 0$, $j = 1, 2, \ldots, m$ and $g_k(x) \leq 0$, $k = 1, 2, \ldots, p$.

However, it is well-known that this formulation succeeds in getting points from all parts of the Pareto set only when the Pareto curve is convex. Das and Dennis provide a graphical interpretation of the weighted sum method for two-objective problems to explain some of its deficiencies.

The second multiobjective technique is the ϵ-constraint method. Haimes et al.[24] introduce the ϵ-constraint approach (also called the ϵ-constraint or trade-off approach), this technique minimizes the single most important objective function f_i, while the $n - 1$ other objective functions are added as inequality constraints of the form $f_q(x) \leq \epsilon_q$ for all $r = 1, 2, \ldots, n$, r i where $i \in 1, 2, \ldots, n$. The vector of upper bounds, $\epsilon = (\epsilon_1, \epsilon_2, \ldots, \epsilon_n)$,defines the maximum value that each objective can have. These inequalities can be interpreted as hyperplanes re- ducing the feasible criterion space. In order to obtain a subset of the Pareto optimal set, one must vary the vector of upper bounds along the Pareto front for each objective, and solve a new optimization process for each new vector. When this multi-objective optimization framework is considered for the MOOP, it can be written as: min f_i, subject to: $f_q(x) \leq \epsilon_q$, $\forall q = 1, 2, \ldots, n$, q i, $h_j(x) = 0$, $j = 1, 2, \ldots, m$, $g_k(x) \leq 0$, $k = 1, 2, \ldots, p$.

Finally, the normal boundary intersection method was developed to overcome the deficiencies related to the weighted sum approach, Das and Dennis[25] presented this method, which provides a means for obtaining an even distribution of Pareto optimal points for a consistent variation in the user-supplied parameter vector w, even with a nonconvex Pareto optimal set. This method essentially works by solving a set of NLPs of the following form:

$$\min_{x,\gamma} \gamma \quad (NBIF)$$

subject to:

$$\begin{aligned} \Phi w + \gamma v &= F(x) - F^u \\ h_j(x) &= 0, \quad j = 1, 2, \ldots, m \\ g_k(x) &\leq 0, \quad k = 1, 2, \ldots, p \end{aligned}$$

Φ is a $n \times n$ pay-off matrix in which the i-th column is composed of the vector $F(x^{*}i) - F^u$, where $F(x^{*}_i)$ is the vector of objective functions evaluated at the minimum of the i-th objective function. The diagonal elements of Φ are zeros; w is a vector of scalars such that $\sum^{n}_{i=1} w_i = 1$ and $w \geq 0$, $v = -\Phi e$, and $e \in R^k$ is a column vector of ones in the criterion space. v is called a quasi-normal vector. Since each component of Φ is positive, the negative sign ensures that v points towards the origin of the criterion space. v gives the NBI method the property that for any w, a solution point is independent of how the objective functions are scaled. As w is systematically modified, the solution to the problem (NBIF) yields an even distribution of Pareto optimal points representing the complete Pareto set.

RESULTS AND DISCUSSION

MODEL FORMULATION

The model is based on previous studies for Larragoiti-Kuri et al., the simulation is made under a sequential modular approach[26,27] on Matlab®, the advantage of using this method is that easily you can add a system in case when the configuration is change. Our simulation follows a description based on deterministic model, and it does not consider uncertainty in the parameters that it uses as average values. Data in the tables consists of average values and are representative of the mexican reality.

A main difference between our study and the previous one from Larragoiti-Kuri et al. is that during the simulation, they consider operation variables and yields previously reported by other authors, and we calculate those yields and variables by including the thermody- namic property functions and kinetic mathematical models, which can find on supplementary information section. Later on, we did a sensibility analysis to select the decision variables that were to be optimized. The premise that was followed to determine whether or not to be considered as a decision variable was that they caused a change of more than five percent on the economical and environmental objective functions, by changing these variables in a range of twenty-five percent up and down from their nominal values. As you can see on the process diagram of the biorefinery in figure 1, the unit operation where nine decision variables are involved, which one are highlight by a black circle. Now we are going to explain each part of the process with special focus on identify where the decision variables are involved.

MASS BALANCE DESCRIPTION

Pretreatment and first stage. The raw material is corncob, firstly it is ground and mixed with sulfuric acid solution for the thermochemical pretreatment where takes place the hemicellulose hydrolysis. In this first stage, it was consider that temperature (T), time of re- action (τ) and acid concentration (C_A) are the most relevant variables that change the yield of hemicellulose to xylose, according to Cai et al. study.[28] Pretreatment stage is one of the most important process in the biorefinery and it has three decision variables for the multiob- jective model. After that, the pretreatment stream product is fed to a press filter, where the fourth decision variable, cake thickness δ, is considered, and which one measures the amount of mass filter on this operation. For compute δ, we have use a polynomial approximation presented by Wakeman in a similar system and it is a function of residence time. [29] After the filtration process, the liquid stream is rich in xylose and the solid one is mainly cellulose and lignin. The liquid one, is used to synthesize xylitol or succinic acid and the solid stream is converted to the other three bioproducts: lignosulfonates, lactic acid and bioethanol. These liquid stream (cellulose and lignin), is feed to a delignification and filtration stages where we have the fifth decision variable, cake thickness δ_2. This liquid stream is rich in lignin and is converted to lignosulfonates, one of the main product from the biorefinery. The solid stream with cellulose can be turned into lactic acid and/or bioethanol, but previously this stream has been neutralized in a batch process to be fed toward the filtration step. Here we have the sixth decision variable beta (β), which is the split fraction stream between lactic acid and bioethanol.

Xylitol and Succinic Acid production. The liquid stream with xylose that comes from the pretreatment, is neutralized in a tank reactor and filtered, then it is fed to an activated carbon column where is detoxified. Then, this single stream is splitting and two product streams are feeding to produce either xylitol or succinic acid. Xylitol is produced by a batch process fermentation, followed by: centrifugation, decolorization, ion exchange and, finally, crystallization processes. These steps are called "XP", as it can be seen in the figure 1. Here we have chosen the seventh decision variable, the filtration yield. For the succinic acid product, a batch process fermentation and a centrifugation are also needed, and it is followed by: decolorization, filtration and cristallization processes. These steps are called "SAP", as it can be seen in the figure 1. And again, we proposed the eighth decision variable (filtration yield).

Lactic Acid and Bioethanol production. After the first stage, following the lactic acid route, is needed a simultaneous, saccharification and fermentation reactor (SSF), here is involved the ninth decision variable (time of reaction). In this part of the process, the lactic acid yield is calculated with an equation presented in the Zhao et al. study [30] for similar systems. After SSF step, a process of separation is need to separate biomass. Then is trans- fered to a tank in order to be neutralized, filtrated, concentrated and, finally, decolorized by a granular activated carbon, where is the tenth decision variable (discoloration yield). For the bioethanol production is needed also a SSF reactor, in this case, the kinetic of the reactor is simulated by the kinetic model of Monod, which is given by an ordinary differential equation for mass balance. We have another decision variable (time of reaction). Effluent is fed to the centrifugation process in order to separate the biomass. Finally, the bioethanol is purified when a distillation and zeolite processes are involved.

Lignosulfonates production. The solid mass fraction from the lignin stream is precipi- tated by acidification with sulfuric acid. Then, solid lignin is fed to a tank reactor, where H_2O_2, $FeSO_4$, CH_2O and Na_2SO_3 are added to generate lignosulfonates. Finally, such product is purified by precipitation and filtration.

ENERGY BALANCE DESCRIPTION

For all the equipment involved in the biorefinery (seventy three), its cost is estimated and that is the initial investment cost (equipment). With this value and fractions related to other fixed costs such as: facilities, pipes, electrical system, buildings, construction expenses, legal expenses, engineering and land, the initial investment cost is estimated.

It is calculated the power of more than a half of the equipment (forty four), and with this value is estimated a part of the variable cost of the utilities, depends on the value of the electricity price. Finally, for thirteen equipment that require cooling water and steam for their duties, we estimated a carbon dioxide emission function by the polynomial fitting. The set of data for curve fitting were generated by Aspen-plus® simulator. we use the utility block to define process heating and cooling utilities and the fuel sources. In this case we chose the natural gas, coal and kerosene, for the steam natural gas and kerosene were chosen but discussion section only the natural gas was considered.

OBJECTIVE FUNCTIONS

Economic Objective Function. The economic aspect is an item that easily indicate the feasibility of the process that is evaluating. The objective economic function, as we mention in the introduction, can be adopted in many different ways but always trying to clearly reflect the economic potential the project has. In our case, it is measure with annual profit of the biorefinery through the following equation:

$$\text{Annual profit} = (\text{revenue} - \text{variable cost})\ \text{batch per year}\ [=]\ kUSD/year \qquad (3)$$

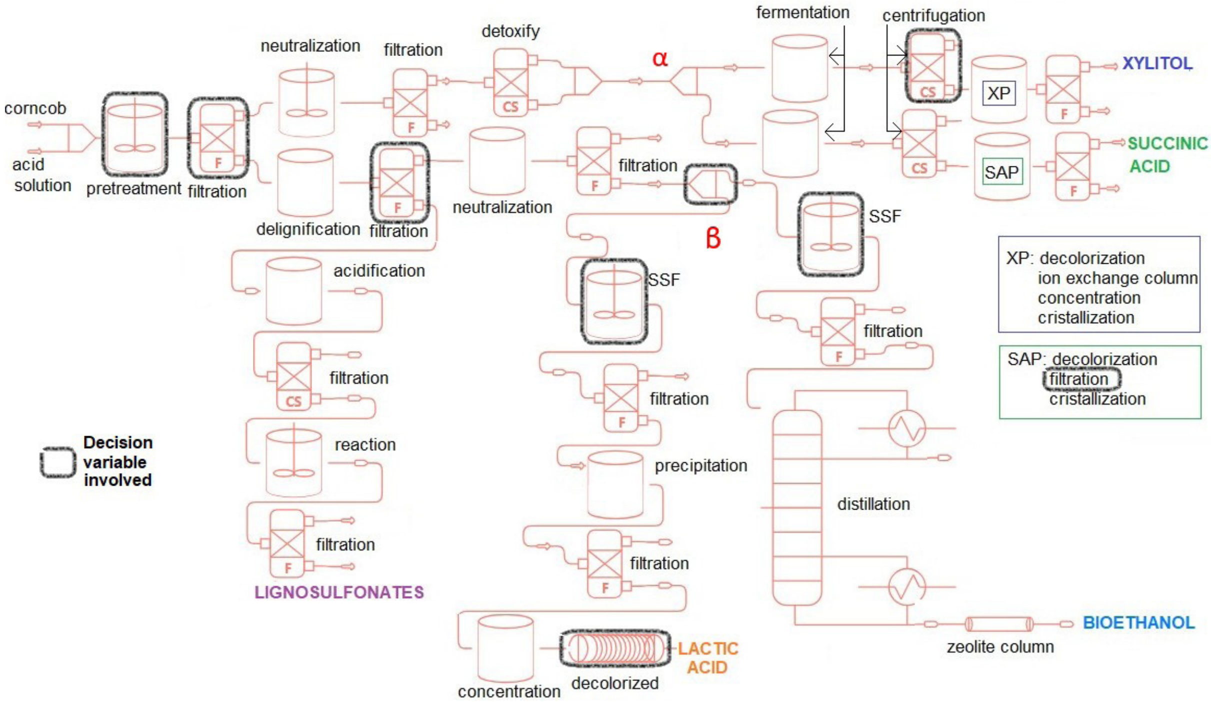

Figure 1: Process diagram in biorefinery

Product	Net imports in Mexico (ton/year)	Production / sales volume (ton/year)	Market share from imports (%)	Delivered price (USD/kg)
xylitol	875	71.1	8.12	4.56
succinic acid	58	0	-	4.27
ethanol	1.2×10^5	457.4	0.004	0.91
lactic acid	7.3×10^3	1.2	0.016	2.43
lignosulfonates	3.7×10^4	61	0.0002	1.0

Table 1: Market size, production volumes and market share from imports.

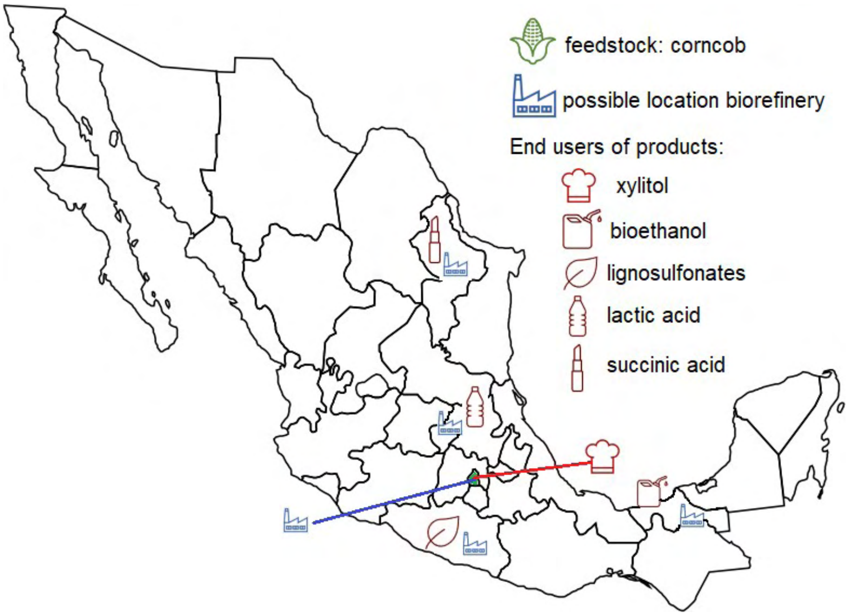

Figure 2: Map of Mexico with possible location of biorefinery and location of end user products

The revenue is calculated with the sum of the products obtained by their sale price, in last column of figure 1 you can see the delivered prices that are considered. To determine the sale price we take into account the import price and only in the xylitol we consider fifteen percent of overprice price because of the price differentiation that customers can pay because this product is made from a clean and novelty technology, unfortunately this overprice is not possible to put on bioethanol, according to Pacini et al. sudy. [31] It is important to mention that we consider in the model a deliver price, and for that reason we need to make an educated guess to the location of final users of the biochemicals that are produced, in the figure 2, it is shown the location of the final users are consider to estimate the transportation cost from the biorefinery to them. The variable cost[32] is the sum of the production costs considering: labor, technical, specialists, maintenance, raw material, services and transportation cost.

Table 1 shows the net imports in Mexico of the five products, the volume of production that results in the efficient solution, the percentage of these volume of sales about the net imports and finally the delivered price that is considered to calculate the revenue (produced volume multiplied by the delivered price).

Environmental Objective Function. We considered the warming global potential as an objective function, where the environmental impact is measured through the CO_2 emissions coming from the heat duty managed carefully in every process stage. The specified results show that both utilities are being used with natural gas, however, the process model has the flexibility of having other fuels such as coal and kerosene, as we explained it in the previous Energy Balance description section.

Social Objective Function. We are interested for providing a perspective on how social concerns can be incorporated in design and analysis operation methodologies for a biorefinery. The considerations presented here deal mainly with a framework that would be useful in incorporating sustainability ideas through the use of appropriate social quantitative metrics. The social objective function was the major contribution in this study because most of others, not consider the social aspect and usually consider only two objective functions instead of three. First of all, we decided to use three key indicators of the social status and condition of a certain location that are reported by National Institute of Statistics and Geographic[33] (INEGI) and those indicators are:

- Crime incidence rate per one hundred thousand inhabitants [*Crime*]
- Complement of the relationship between occupation and working-age population [*Unemployment*]
- Social Lag Index, this indicator includes social deprivations in: education, health, basic services, quality and spaces in home, even assets in home [*Social lag*].

Three indicators where normalized and then related to construct one factor according with the following equation:

$$\textit{Social index factor} = w_{cr}\,[\,\textit{Crime}\,] + w_{un}\,[\,\textit{Unemployment}\,] + w_{lag}\,[\,\textit{Social lag}\,] \quad (4)$$

where the weights of crime, unemployment and social lag factor are: w_{cr}, w_{un}, w_{lag}, respectively, and which ones have to satisfied the equality constraint $w_{cr} + w_{un} + w_{lag} = 1$.

As you can see, the three indicators reflect negative social items in a society, so, we want that this indicator was minimized in order to reflect and improve on the society we are evaluating. In the current study the values of the weight factors were: 0.3, 0.3 and 0.4, respectively.

It is calculated the social index factor for the 32 states in Mexico, then are sorted and selected five possible locations across Mexico, all of them where scattered with all of the possible values of the factor. In the figure 2 are shown the five possible location in a map of Mexico for better visualization.

These five possible locations found are: (1) Nuevo Le´on, (2) Ciudad de México, (3) Querétaro, (4) Tabasco and (5) Guerrero. Each location has different population, so we proposed a method to relates the quantity of new employees (direct and indirect) generated with the biorefinery to obtain what we called "improvement value" and then a new value of original three indicators. Later, we calculated again the "new" social index factor and we measured the percentage of improvement. The number of direct employment is calculated according to Peters et al. and depends on the equipment.[32] It is considered three shifts per day. The indirect jobs are calculated depending on direct ones and according to the relationship (0.9754 direct/indirect employments) valid for biofuels according to Institute for Diversification and Energy Saving.[34] Due to nature of the process and the small scale of the biorefinery, it is found a relation of 0.338 employments/tons of products, this value bigger that the reported on Miret et al. of 0.008 employments/tons of products and the reason of the difference is mainly the scale of production, in the biorefineries reported in Miret et al. study, are produced 400,000 ton/year and in the one we optimized, around 600 ton/year.

SIMULATION AND OPTIMIZATION RESULTS

Before the optimization study, the biorefinery simulation is performed. The model has the flexibility to update the raw materials and final products prices easily and according to the market requirement. Then, the sensitivity analysis over the multiobjective optimization problem has been performed varying the split fraction (α) to produce either xylitol or succinic acid. To do this the normal boundary intersection method (NBI) is employed in Matlab®, which the limits of the variables were imposed as inequality constraints.

The objective functions response are shown in Figures 3, 4 and 5 for different values of the split fraction α. The feasible lower bound found for α was 0.7, although succinic acid and xylitol delivered prices are alike. These figures show the Pareto frontier for each couple of the objective functions: social, economic and environmental aspects. The theoretical economic equilibrium can be seen in figures 3 and 4 (solid vertical line) where the combination of economic variables, prices and quantity products and raw material, shows the feasible region to find the optimal solutions and it drives the economy of the biorefinery. In figure 3 can be noticed that along the economic equilibrium line the quantity of CO2 produced do not represent differences larger than 44%, while in figure 4, the social benefit differences are smaller than 17% when the split fraction for succinic acid and xylitol is varying from 0.8 to 1.0.

The compromise solution is summarized in table 2 and the eleven decision variables for the efficient solution are also summarized in the table 3. In this case, Tabasco has the best economic value but we have chosen Querétaro because its social benefit value is better than the first one. In other simulations, the social benefit is higher most of the times in Querétaro, however, the economic benefit for small values of alfa is in favor of Tabasco, for medium values of alfa is between Mexico City, Querétaro and Tabasco, and with high values of alfa preferred Mexico City. The efficient solution for product distributions are depicted from the figures 6 to 8 and they are compared against Larragoiti work. All of the optimum flow rates have decreased, for instance: xylitol, lignosulfonates, succinic acid and lactic acid on 34.6%, 5.8%, 100% and 91.3%, respectively, whereas the bioethanol has increased on 53.3%.

The annual profit is bigger than the previous work of Larragoiti-Kuri et al. in the same biorefinery, where it was 71.9 kUSD,[2] the difference is mainly the actualization of the product prices and the different configuration and volumes of products that were produced. In the study of Yeh et al., the biorefinery produces gasoline from other source and with more capacity of production (140 kton of product), the profits they report in some price level are around 250 million dollars, so they have a profit per ton produced of 1714.3 USD/ton.[16] In our study, this value is 347.5 USD/ton produced. We attribute the difference to the scale of the biorefinery we are simulating. Because the present comparison refers to the five main products with a corncob raw material only, a complete life-cycle analysis should be performed to obtain a complete cradle-to-grave assessment of the biorefiney. However, the results provide interesting insight into a potential opportunity to take advantage of residue of maize crop. In general, all of the objective functions hit the efficient value of each sustainable indicator. The combination of such metrics provides an convenient evaluation of the operating conditions.

CONCLUSIONS

The results of the simulation and the multi-objective optimization problem we present, show us the optimal operating policy and also the recommended location to the lignocellulosic biorefinery. It is important to mention that the model we develop has flexibility to easily change some indicators such as the weight of the three factors we use in the social objective function, the prices of the raw material or the sales price, among other. Several studies that evaluate the social benefit of a process, did it by estimate the number of employments that generate, just like Miret et al..[8] In our work, we also estimate the generation of jobs and not only the direct employees but also the indirect ones. Because of the configuration of the biorefinery, the number of jobs generated is variable and depends on the results of the optimization, so we relate this variable with public information related to social aspects and quantify the social benefit. The location of the biorefinery that result in the efficient solution is in the city of Queretaro, near Mexico City. Further work can explore social aspect and consider not only the number of generated jobs but also the interest of the stakeholders involved in the process. Finally, this work may be extended to consider uncertainty and stochastic versions of the model.

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Objective function	Variable	Value	Units
Economic	Annual Profit	205	kUSD/year
Environmental	CO_2 Mass	166.6	ton/year
Social	Social benefit improvement	13.72	%

Table 2: NBI optimization results for the objective functions.

Number	Variable	Value	Units	Stage
1	Temperature (T)	110	ºC	Pretreatment
2	Time of reaction (τ)	0.7	h	Pretreatment
3	Acid concentration (C_A)	0.7	%w/w	Pretreatment
4	Cake thickness (δ)	10	cm	Detoxify
5	Cake thickness (δ_2)	49.98	cm	Delignification
6	Split fraction (β)	0.0096	-	Delignification
7	Filtration yield	0.049	-	Xylitol production
8	Filtration yield	0.152	-	Succinic acid production
9	SSF time	10.48	h	Lactic acid production
10	Discoloration yield	0.9936	-	Lactic acid production
11	SSF time	15	h	Bioethanol production

Table 3: Values and stage of decision variables.

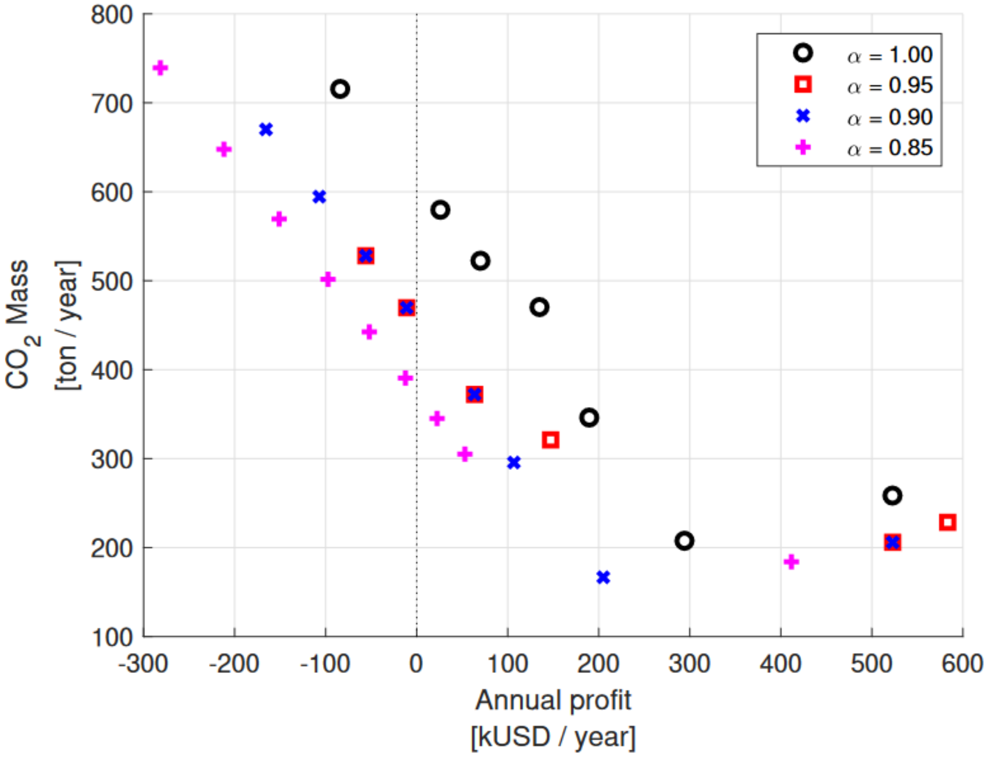

Figure 3: Pareto frontier for environmental and economic objective functions for different values of α to produce either xylitol or succinic acid, and (· · ·) economic equilibrium line.

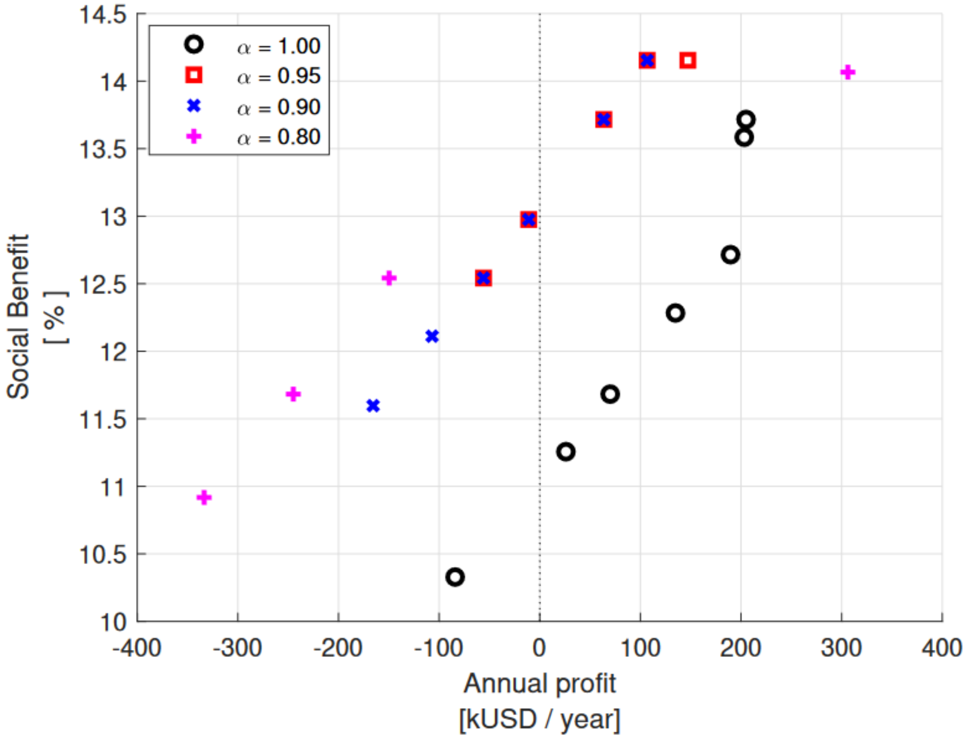

Figure 4: Pareto frontier for social benefit and environmental objective functions for different values of α to produce either xylitol or succinic acid, and (· · ·) economic equilibrium line.

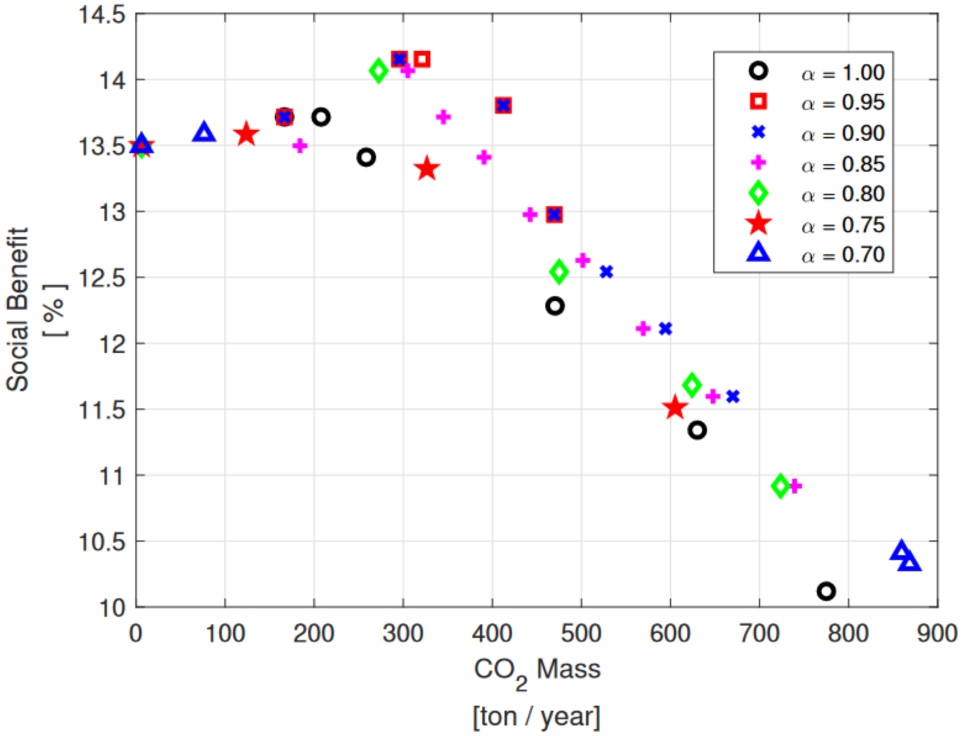

Figure 5: Pareto frontier for social benefit and economic objective functions for different values of α to produce either xylitol or succinic acid.

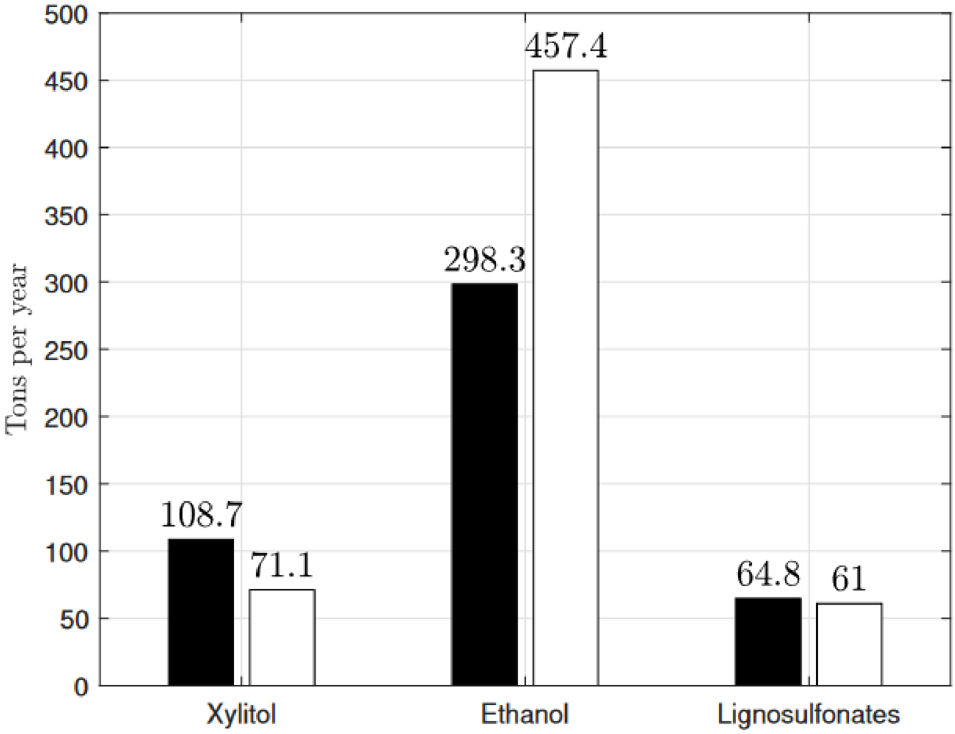

Figure 6: Product Distribution for: (a)Xylitol, Ethanol and Lignosulfonates, the white columns are for this work while black ones are for Larragoiti's one.

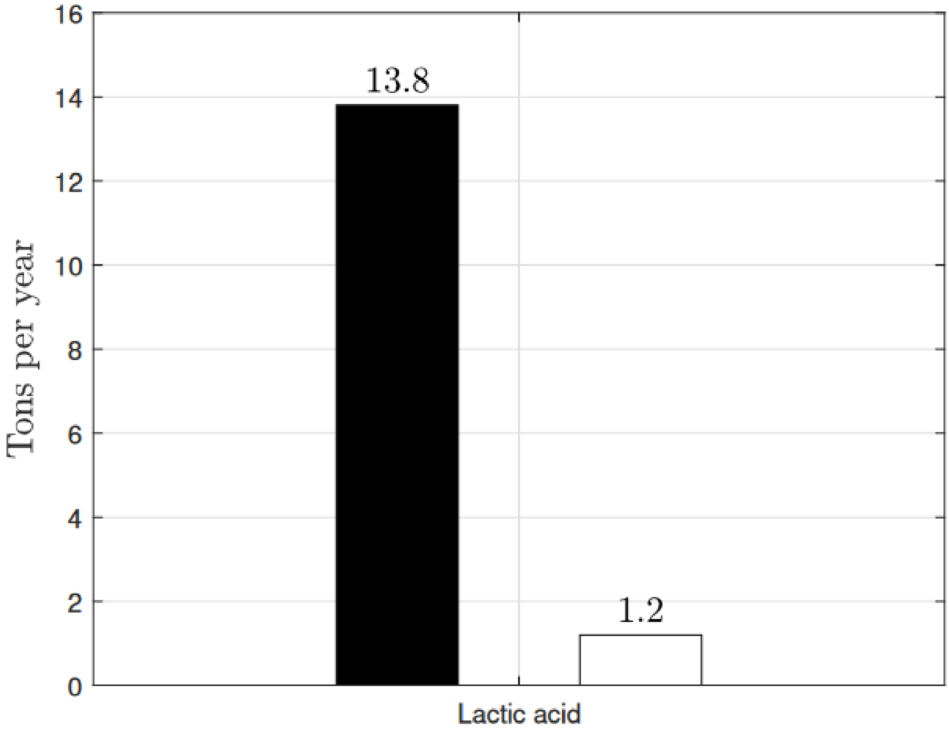

Figure 8: Product Distribution for Lactic acid, the white columns are for this work while black ones are for Larragoiti's one.

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