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An MILP model to identify optimal strategies to convert soybean straw into value-added products

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ABSTRACT

Soybean is a highly valuable global commodity due to its versatility and numerous derivative products. During harvest, all non-seed materials become “straw”. Currently, this waste is primarily used for low-value purposes such as animal feed, landfilling, and incineration. To address this, the present work proposes a conceptual biorefinery aimed at converting soybean straw into higher-value products. The study began with data collection to identify potential conversion routes. Based on this information, a superstructure was developed, comprising seven conversion routes: four thermochemical routes (pyrolysis, combustion, hydrothermal gasification, and liquefaction), two biological routes (fermentation and anaerobic fermentation), and one chemical route (alkaline extraction). Each process was evaluated based on product yields, conversion times, and associated capital and operating costs. Using this data, an MILP (Mixed-Integer Linear Programming) optimization model was built in Pyomo using CPLEX as the solver. The variables in this problem were the amounts of biomass processed by each conversion process. The objective function was to maximize the Net Present Value (NPV). The optimization considered a maximum raw material supply of 232,500 metric tons per year. As a result, pyrolysis was identified as the most profitable route, yielding US$447 million, producing biochar, bio-oil and gas as products. It was observed that only if the price of the optimum product was 46% lower would the optimum conversion process change. In conclusion, soybean straw offers significant potential for value-added applications in a biorefinery context, with pyrolysis emerging as the most profitable route.

Keywords: Optimization, Pyomo, Biomass, Soybean, Biorefinery

INTRODUCTION

Since the Industrial Revolution, petroleum, coal and natural gas have been the primary energy sources. Technical achievements have come with the use of these energy sources, *e.g.*, developing steam engines, chemical products and fuels. However, oil has a depletion time of less than 270 years and takes approximately about 280 million years to regenerate [1]. Moreover, the exploitation of fossil fuels has a significant impact on the environment, including soil and water contamination and the release of harmful gases that intensify global warming [2]. Given this context, it is necessary to find different sources that have less environmental and social impacts.

Lignocellulosic biomass is one of the most promising alternatives to fossil fuels due to its large availability. In addition, its structure is complex, consisting of four different organic compounds (cellulose, hemicellulose, lignin and extractives) and one inorganic component (ash), which can produce a substantial number of different value-added products with high energy potential. The renewable nature of lignocellulosic biomass stems from the fact that the CO_2 produced when burning biomass is reabsorbed by plants during their development, maintaining a carbon-neutral cycle [3]. Various processes that modify biomass structure and generate new products have been studied over the years.

To develop sustainable and profitable production systems, large amounts of data are necessary, which can sometimes become intractable to analyze. From a process systems engineering (PSE) perspective, computation tools are recommended because analyzing vast amounts of data from different sources manually is challenging [4]. Techno-economic optimization can reduce costs in the initial stages, particularly in process systems with significant uncertainties, such as biorefineries

Biorefinery is an integrated industrial process that incorporates individual units that convert biomass into power, biofuels and value-added chemicals. The conversion process used in biorefineries can be divided into four principal groups: mechanical processes (size reduction, separation and concentration of substances); thermochemical processes, (pyrolysis, gasification, liquefaction and combustion); biological processes (fermentation and anerobic fermentation); and chemical processes, which use chemicals to change the structure of the input material [5].

Table 1 – Production of soybean by country/region in 2022/23 [6]

	Production (MMT)	World Share (%)[1]
Brazil	162	42,9%
United States	116	30.7%
Europe	2.61	0.69%
World	378	100%

[1] Country/Region production as a percentage of world production

Brazil is the largest producer of Soybean (*Glycine max)*, followed by the United States, collectively, they represent over 70% of global production (Table 1). With all this crop, a lot of waste is generated, the principal one is soybean straw, composed of leaves, steams and pods with lignocellulosic composition of 35% of cellulose, 22% of lignin, 17% of hemicellulose and 1% of ashes [7]. It is estimated that the ratio of straw to soybeans varies from 1.2 to 1.5 [8], which represented, in 2023, 194.4-243 million metric tons of waste. Most of the straw is used as landfill, livestock feed, incineration or dumping [7, 8].

Considering those known destinations, soybean straw does not have nutritional value compared to other crops residues *e.g.*, sorghum or corn, to be used as animal feed. However, it is necessary to keep part of the straw in the land to protect the soil from runoff, infiltration and soil loss. The Brazilian Agricultural Research Corporation (EMBRAPA) [9] estimated that it is necessary to keep 2.205 metric ton per ha to protect the soil, so almost 50% of all soybean straws needs to be used for landfill, in the context of Brazilian scenario.

Given the lack of current uses, the large availability and its lignocellulosic composition, soybean straw has a lot of potential to produce chemical products and fuels. The objective of this work was to develop a superstructure of a conceptual soybean straw biorefinery and solve it using an MILP (Mixed Integer Linear Programming) optimization, with Net Present Value (NPV) as the objective function.

METHODOLOGY

The methodology was based on three steps. The first one was a literature review, which was necessary to find conversion processes and products that can be obtained from soybean straw. The second one was data treatment, to standardize the data, making it possible to use it in a generic framework. The final step was the development and solution of an MILP optimization model.

Literature Review

All chosen products and their respective process routes for soybean straw valorization were gathered from academic literature.

Process costing was performed using similar routes reported in literature. There were two types of cost considered: a capital cost (CAPEX), which considers equipment, installation and instrumentation cost; and an operating cost (OPEX), which covers the reactants' price, labor charges and other administrations costs. For all the selected products, a revenue price was determined. While some have a known market price, others had to be estimated.

Data Treatment

The basic premises considered were: 350 days a year as operating time; 2023 as the reference year; the biomass availability as all soybeans straw waste in the city of Itapeva, São Paulo State, in 2023 (232,500 metric ton) [10]; 10 years of plant lifetime operation; no cost associated with the feedstock; and a discount rate of 12.25% per year.

The yield of each product was adjusted to be per gram of biomass. Because it was used an annual biomass availability, it was necessary to find an annual yield of each product, so, the conversion time of each process was considered.

In Eq. 1, CAPEX was adjusted by capacity and time using a power-law expression [11], where A is the capacity of this biorefinery (27.68 MT h^{-1}); $CAPEX_{ref}$, $CEPCI_{ref}$ and A_{ref} are the CAPEX, Chemical Engineering Plant Cost Index and plant capacity, in t h^{-1}, found in the articles for each route, respectively [21-28].

$$CAPEX = CAPEX_{ref} \cdot \left(\frac{CEPCI_{2023}}{CEPCI_{ref}}\right) \cdot \left(\frac{A}{A_{ref}}\right)^{0.67} \tag{1}$$

OPEX was adjusted, as well, using Eq. 2.

$$OPEX = OPEX_{ref} \cdot \left(\frac{CEPCI_{2023}}{CEPCI_{ref}}\right) \cdot \left(\frac{A}{A_{ref}}\right) \tag{2}$$

It was not possible to find the market price for some products. In such cases, two approaches were used to determine the price: comparing the function of the product (*i.e.*, the price of biochar produced in a pyrolysis route was estimated using coal as reference, using the low heating value as comparison parameter), or similarity

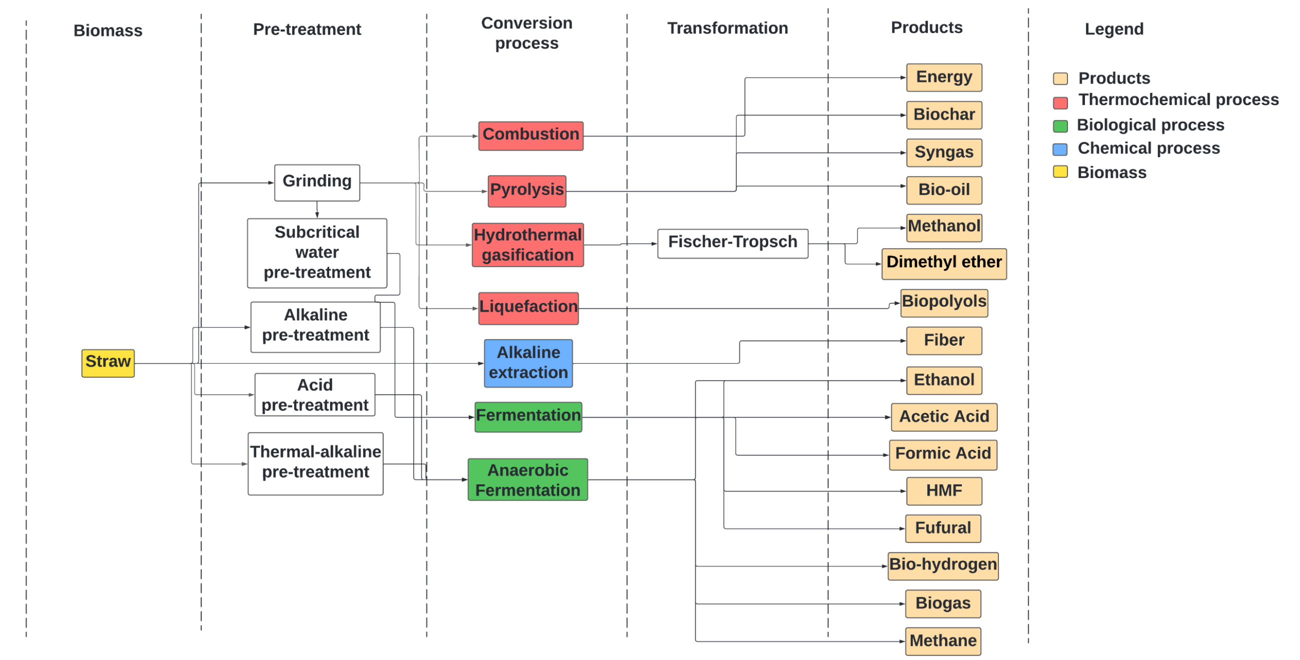

Figure 1: Superstructure for soybean straw valorization

with products commercially available (*i.e.*, the price of pulp and polyurethane was used as the price of fiber and biopolyols produced from soybean straw, respectively).

MILP Optimization

For the MILP optimization, the capital letters represent the parameters and the small ones, the variables. The objective function (Eq. 3) was the maximization of the Net Present Value (NPV), where R represents the discount rate; *i* , *j* and *t* are the sets for processes, products and lifetime, respectively; $N_{i,j}$ represents the yield of each product *j* in the process *i*; P_j is the price of the product *j*; d_i is the non-negative variable, representing the amount of soybean straw used in the conversion process *i* ; C_i and O_i represents the CAPEX and OPEX for the process *i*, respectively, and y_i is the binary variable to decide what process *i* will be selected.

$$\max NPV = \sum_{t=0}^{10} \frac{\sum_i \sum_j N_{i,j}.P_j.d_i - \sum_i O_i.y_i}{(1+R)^t} - \sum_i C_i \cdot y_i \quad (3)$$

The constraints used were:

A big-M constraint to represent the upper bound of the variable d_i and the activation of the binary variable y_i(Eq. 4);

$$d_i \leq y_i.D \quad (4)$$

The total biomass used in all processes is equal to the total available biomass (*D*) (Eq. 5);

$$\sum_i d_i = D \quad (5)$$

An anaerobic fermentation route includes two distinct pre-treatments; therefore, an additional constraint (Eq. 6) was required to prevent them from being selected simultaneously. The subindexes (6.1, 6.2) follow the numbering adopted in Table 2 for the conversion processes.

$$y_{6.1} + y_{6.2} \leq 1 \quad (6)$$

The model was solved using Pyomo (a Python-based, open-source optimization modeling language). The solver used was CPLEX, which uses the "branch and bound" or "branch and cut" methods [12].

Sensitivity Analysis

A sensitivity analysis was conducted to evaluate the impact of various uncertainties. Specifically, the market prices of the products associated with the optimal route were varied within a range of -60% to 30%. This analysis aimed to assess how the objective function and the decision variables are affected by these changes.

RESULTS AND DISCUSSIONS

Literature Review

Four thermochemical processes (pyrolysis [13], liquefaction [14], combustion [15], and hydrothermal gasification [16]), two biological processes (fermentation [17] and anaerobic fermentation [18, 19]), and one chemical (alkaline extraction [20]) were selected. Thus, the superstructure covers the main types of conversion routes.

Figure 1 represents the superstructure created. There were sixteen products found (biochar, bio-oil,

Table 2: Reference and calculated capital and operated costs per conversion process

	Conversion process	$Capacity_{ref}$ (MT h^{-1})	$CAPEX_{ref}$ (M US$)	$CAPEX_{calc}$ (M US$)	$OPEX_{ref}$ (M US$ yr^{-1})	$OPEX_{calc}$ (M US$ yr^{-1})	Ref.
1	Pyrolysis	1.25	0.980	10.4	0.115	3.39	[22]
2	Fermentation	83.3	69.0	45.1	198	90.1	[23]
3	Liquefaction	2.19E-05	0.019	226	0.0004	548	[24]
4	Alkaline extraction	17.3	469	631	8.37	13.1	[25]
5	Anaerobic Fermentation	29.4	70.0	94.9	44.4	59.0	[26]
6.1	Anaerobic Fermentation[1]	0.005	0.299	132	0.078	596	[27]
6.2	Anaerobic Fermentation[2]	0.005	0.299	132	0.078	595	[27]
7	Combustion	0.206	0.333	12.5	0.113	21.4	[28]
8	Hydrothermal gasification	36.6	5.98	4.96	0.204	0.154	[21]

[1] Alkaline pre-treatment
[2] Acid pre-treatment

syngas, methanol, dimethyl ether, biopolyols, fiber, ethanol, acetic acid, formic acid, hydroxymethyl furfural - HMF, bio-hydrogen, biogas, and methane). For the hydrothermal gasification, it does not have the Fischer-Tropsch transformation process. This route was proposed to diversify the products and to facilitate the pricing of the syngas [21].

Table 3: Yield of products for different conversion processes

Process	Product	Yield ($g_{biomass}^{-1}$)
1	Biochar	0.220 g
	Bio-oil	0.720 g
	Gas	0.060 g
2	Ethanol	0.279 g
	Acetic Acid	0.087 g
	Formic Acid	0.052 g
	HMF	0.001 g
	Furfural	0.001 g
3	Biopolyols	0.650 g
4	Fiber	0.250 g
5	Methane	194 mL
6.1	Bio-hydrogen	3.14 mL
	Ethanol	0.006 g
	Acetic Acid	0.019 g
6.2	Bio-hydrogen	47.7 mL
	Ethanol	0.001 g
	Acetic Acid	0.019 g
7	Energy	0.005 kWh
8	Methanol	0.071 g
	Dimethyl ether	0.051 g

Data Treatment

Table 2 has all the associated costs for each process. It is possible to observe, when CAPEX and OPEX were adjusted for the capacity of the biorefinery studied, thermochemical processes had lower costs when compared to biological and chemical processes, especially because almost no auxiliar materials (such as chemicals) are used.

Table 3 shows the yield of products for different conversion processes. It is possible to conclude that for the same route a change in the pre-treatment can significantly impact on the yield of some products (*e.g.,* bio-hydrogen). Moreover, when using aerobic microorganisms, a larger amount of ethanol is produced than when using anaerobic ones. In biorefinery context, even if inhibitors are produced (HMF and furfural) in a fermentation route, revenue is still obtained, and sometimes, this product can be transformed and have a higher market price than the main product. Furfural, for instance, is a chemical platform from which a lot of other chemicals can be derived from.

MILP Optimization

For the MILP model, nine decision variables were considered with ten constraints. The objective function resulted in an NPV of US$447 million, selecting the pyrolysis route as the optimum route, producing biochar, bio-oil and gas.

Figure 2 illustrates the NPV of each process route evaluated. Three of the evaluated thermochemical routes were the most profitable, and only the thermochemical routes led to positive values for the objective function. This could be explained by the biomass chemical composition, as identified in the studies by Eason and Cremaschi [29], lignocellulosic waste (*e.g.*, switchgrass) is most efficiently utilized through thermochemical processes. In contrast, certain grains or seeds, which contain significant amounts of oil and starch, are better suited for valorization through transesterification or fermentation.

The NPV of the most profitable route, pyrolysis, is twice as high as that of the second most profitable route (*i.e.* combustion). It is known that pyrolysis process has a low TRL (Technology Readiness Level) compared with other thermochemical routes, mostly because of the high complexity kinetics of this process creating some uncertainties. Alternatively, combustion is a well-developed process, which could be an interesting alternative for the pyrolysis process for this case.

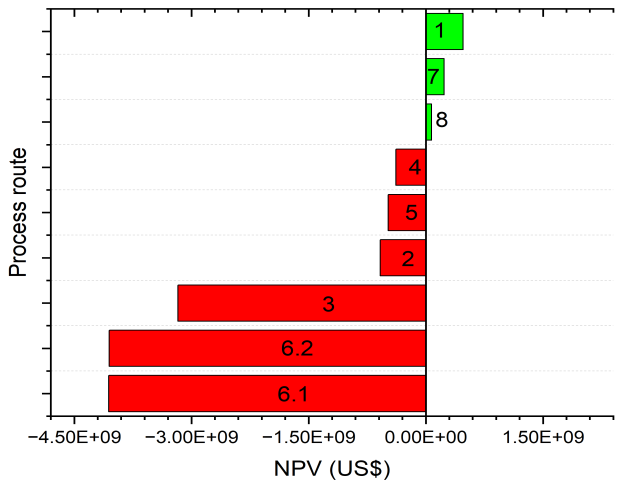

Figure 2: NPV value for each process route

Sensitivity Analysis

The profitability of pyrolysis remains robust despite price fluctuations. In Figure 3, it was observed that it is necessary a 46% decrease in these products' price for the pyrolysis route to be substituted by the combustion as the best route. These two thermochemical routes have very profitable products and lower costs, which justify these optimum results.

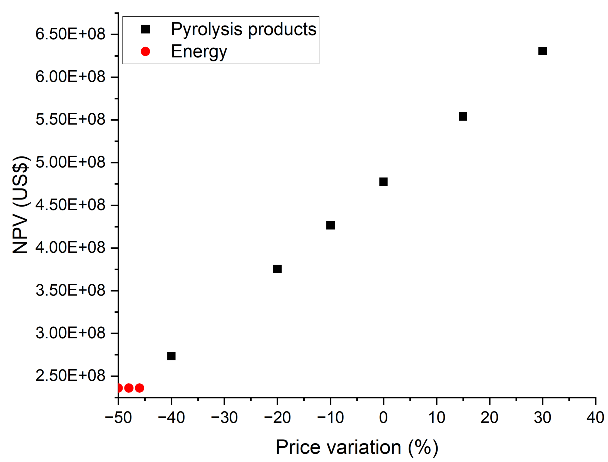

Figure 3: Effect of optimal product price variation on the objetive function

Fischer-Tropsch products are frequently cited as playing an important role in future biorefineries. To produce methanol and dimethyl ether in this biorefinery and keep almost the same profit as the optimum one, it will be necessary that the price of these products increases 6.5 times. This analysis shows that it is unlikely that Fischer-Tropsch chemicals could be profitable at least in the short term in a soybean straw biorefinery.

CONCLUSION AND NEXT STEPS

A conceptual biorefinery using soybean straw as feedstock can be profitable. Pyrolysis emerged as the optimum route, generating biochar, bio-oil and syngas as products. The second-best route for soybean straw valorization was combustion. The optimum products demonstrated a resilient price market, although the technology has a significant associated uncertainty. Evaluating this biorefinery could foster sustainable industrial development by valorizing agricultural waste, serving as an initial study to further evaluate different supply combinations, operational conditions, or end-product prices.

Future research will focus on calculating equipment sizes to refine CAPEX and OPEX estimates. Moreover, the influence of other parameters (*e.g.*, feedstock cost variations, discount rate changes, and OPEX fluctuations) will be investigated to better understand the behavior of the decision variables. A multi-objective and multi-feedstock approach will also be considered to assess the environmental and supply chain aspects.

DIGITAL SUPPLEMENTARY MATERIAL

A supplementary material is available in LAPSE:2025.0034 with the data extracted, from the literature review, and treated to model the optimization.

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