A NEW MILP-BASED SUPERSTRUCTURE FOR BIOREFINERY OPTIMIZATION CONSIDERING HEAT INTEGRATION – A SUGARCANE BIOREFINERY CASE STUDY

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ABSTRACT

In this work, a new MILP-based superstructure formulation is presented to determine an optimal biorefinery configuration, considering process selection and scale-up, and simultaneous utility selection and heat cascade integration. The formulation is used to study the integration of different biofuels production in a sugarcane biorefinery. The conventional ethanol production had the lowest payback, while methanol production by bagasse gasification, the lowest total annualized cost. The results indicated that heat integration is crucial to make bagasse available for biofuel production, improve biorefinery energy efficiency, and increase its revenues. Furthermore, the price of electricity can be seen as a bottleneck in integrating methanol production through the CO_2 conversion route.

Keywords: MILP-based superstructure, Sugarcane biorefinery, Heat cascade integration, Biofuels.

Introduction

The production of biofuels in biorefineries is crucial for the development of a low-carbon economy. However, the industry is still small because of the low competitiveness of the products, necessitating the development of more efficient processes. Process heat integration is a tool that aims to identify heat exchange opportunities between processes to reduce CO_2 emissions and fuel consumption, thus enhancing energy efficiency [1]. The development and optimisation of biorefineries using superstructures has grown. Employing Mixed Integer Linear Programming (MILP) methods, the superstructures are capable of systematically generating and evaluating all configurations that a set of processes can present. In literature, it is already possible to find works that implement energy integration methods in superstructures, as Celebi et al. [2], that proposed a multi-objective methodology to compare process in different conversion routes in a lignocellulosic biorefinery, and Gassner et al., [3] that optimized the lignocellulosic biomass conversion into liquid fuel. Despite this, from the works found, the authors use a sequential approach to solving the superstructure when they include energy integration or aim to optimize the utility system, which can result in a high computational cost, in addition to non-optimized configurations. Therefore, this work aims to present a new MILP-based superstructure formulation capable of performing process selection and scale adjustment simultaneously, in addition to energy integration and utility selection. It is used to assess the effects of integrating other biofuel production in a sugarcane biorefinery.

Methodology

The superstructure is made up of mass and energy balance constraints, based on the work of Kantor et al.[4], while the heat cascade constraints are based on Bagajewicz M. and Rodera [5]. The MILP formulation was developed and implemented through the LINGO software, and all the constraints are solved simultaneously, ensuring that a global optimum is obtained.

A. Superstructure Mass Balance and Objective Function Formulation

Each process in the superstructure has its scale divided into levels, which are intervals limited by a maximum and minimum value. Each of these levels ensures that scale adjustment occurs linearly within that range. The selection and scale adjustment of each process u, is carried out by equation (1), where $CapMin_{u,l}$ and $CapMax_{u,l}$ are parameters that represent the maximum and minimum scale adjustment that a process can have in a certain level l, $y_{u,l}$ is a binary variable that represents the existence of that unit in that level, that assumes 1 if the unit is selected or 0 otherwise. Each process can only have up to one level selected. $wl_{u,l}$ is a continuous variable responsible for the process scale adjustment into that level, while w_u is a continuous variable that represents the scale adjustment for that process. The superstructure mass balance is performed by equation (3), where $bought_r$ and $sold_r$ are continuous variables representing the quantity bought and sold of resource r, and fop is the time that this process operates in a year. $IAR_{u,r}$ and $OAR_{u,r}$ are the consumption and production of a resource r in a process u.

$$CapMin_{u,l} \cdot y_{u,l} \leq wl_{u,l} \leq CapMax_{u,l} \cdot y_{u,l} \tag{1}$$

$$\sum_{l} wl_{u,l} = w_u \tag{2}$$

$$bought_r + \sum_{u} OAR_{u,r} w_u fop = \sum_{u} IAR_{u,r} w_u fop + sold_r \tag{3}$$

The superstructure's objective function, stated in equation (4), aims to minimize the total annualized cost (TAC) by factoring in investment and resource acquisition expenses, along with revenues generated from carbon credits and resource commercialization, as presented by equation (5). Equation (6) provides the annualized investment cost of a unit u (AIC_u), where $a_{u,l}$ and $b_{u,l}$ represents the variable and fixed cost, respectively, of a process *u* presents in a level *l*. Equations (7) and (8) are used to calculate cost and revenue with resource r, where $ResCost_r$ and MP_r represent the cost and market price of resource r, respectively. Carbon credit revenue is calculated by equation (9), which considers the amount of CO_2 emitted and avoided by a given resource, denoted as $EmittedCO2_r$ and $AvoidedCO2_r$ respectively. CarbVal represents the carbon credit market price.

$$Objective\ function = \min TAC \tag{4}$$

$$TAC = \sum_{u} AIC_u + \sum_{r} RC_r - \sum_{r} PC_r - CC \tag{5}$$

$$AIC_u = \sum_{l} (a_{u,l} wl_{u,l} + b_{u,l}\, y_{u,l}). AF. (MC + OC + LC) \tag{6}$$

$$RC_r = Bought_r ResCost_r \tag{7}$$

$$PC_r = Sold_r MP_r \tag{8}$$

$$CC = \left(\sum_{r} Sold_r AvoidedCO2_r - \sum_{r} Bought_r EmittedCO2_r \right) CarbVal \tag{9}$$

B. Heat cascade integration and utility selection

Utility selection constraints identify the stage in a heat cascade at which a utility can supply heat and is limited to its quantity demanded. For that, the method considers the inlet and outlet temperatures of each stage, as well as the utility temperature. Likewise, energy integration constraints between cascades identify temperature ranges in which two processes can exchange heat. This region is limited to the cascade stages located between the pinch temperatures of each process. The amount of thermal energy that a process can receive, whether in the form of utility or through integration with other processes, is determined by equation (10), where MER_u is the Minimum Energy Requirement of an process, and UF_u is its cold utility consumption. Qin_u and $Qout_u$ are the heat received and donated to others process by heat cascade integration, while $Qut_{ut,u}$ is the energy consumed as utility.

$$
\begin{aligned}
w_u MER_u &= \sum_{ut} Qut_{ut,u} + Qin_u \\
w_u UF_u &= \sum_{ut} Qut_{ut,u} + Qout_u
\end{aligned}
\qquad (10)
$$

Case study

The presented formulation was used to evaluate the impact of different biofuels production in a sugarcane biorefinery. In this sense, different processes were included into the biorefinery as black-box models. Five different cases were considered and presented in Table 1. The first case aims to represent the conventional distillery, while case 2 evaluates the integration of vinasse biodigestion with biomethane production. Case 3 e 4 evaluates the methanol production by bagasse gasification integrated to methanol production, and Carbon Dioxide Catalytic Hydrogenation process, respectively. The last considers the CO2 produced during the juice fermentation process. Case 5 evaluates the integration of the methanol catalytic dehydration process, which converts methanol to DME.

Table 1 – Cases and its evaluated routes.

Case	Biofuel	Route	Source
1	Ethanol	Destillery	[6]
2	Methane	Vinasse Biodigestion	[7]
3	Methanol	Bagasse Gasification	[8]
4	Methanol	Carbon Dioxide Catalytic Hydrogenation (CCH)	[9], [10]
5	DME	Methanol Catalytic Dehydratation (MCD)	[8]

For utilities production, three cogeneration systems were considered, producing saturated steam at 2.2, 6 and 9 bar pressure, and electricity. EES software was used to model these systems, using bagasse as fuel and assuming a cogeneration efficiency of 85%. Alkaline electrolysis was used to produce hydrogen (H_2), as required in case 4. Furthermore, the generation of electricity by a system of photovoltaic solar panels was considered and an availability of 2,640,000 tons of sugar cane. For the sale of carbon credits, the price of $ 65.00. Figure 2 shows the processes included in the superstructure.

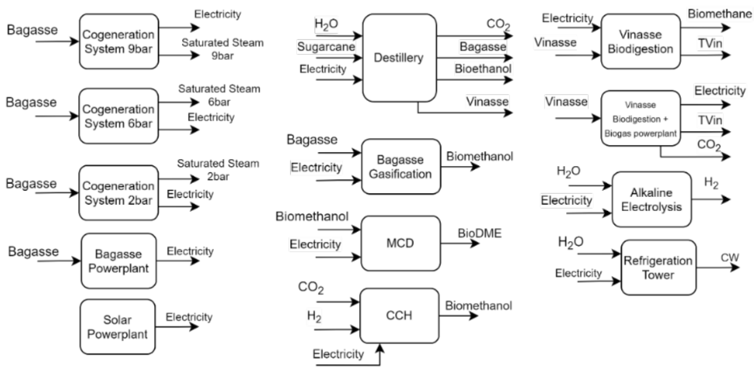

Figure 1 – Representation of the process included in the superstructure.

Results

With the superstructure solution for each case, it was possible to calculate the payback and energy efficiency of each case, as shown in the Table 2. For case 1, the configuration presented is close to a conventional distillery in Brazil, with a cogeneration system that produces saturated steam at 6 bar. In this case, surplus bagasse is sent to a bagasse powerplant, which sells surplus electricity. In case 2, the vinasse biodigestion process, resulted in a TAC reduction and energy efficiency improvement. As the biofuel production is increased, its revenues and energy production also increase, improving its energy efficiency. In case 3, the joint production of methanol and ethanol considerably increased the energy efficiency of the biorefinery while also increasing the payback. Despite the greater investments required, the bagasse gasification process uses a large amount of heat for energy integration, to meet its own demands and those of the biorefinery. In this way, all the bagasse generated can be transferred to gasification without compromising the heat supply to the processes. To meet electricity consumption, the biorefinery used a photovoltaic panel system to generate electricity. Initially, methanol production via the CCH route in case 4 proved to be unfeasible. By forcing production through this route to consume all the carbon dioxide released by the distillery, the biorefinery presented a TAC of $6{,}503 \times 10^7$ and a payback of -18.26 years. When biorefinery expenses were evaluated, a high cost associated with hydrogen production was observed, mainly related to its high electricity consumption. To verify the cost impact associated with hydrogen production, it was considered that the biorefinery could import green hydrogen at a cost of 3.5$/kg. As a result, the biorefinery presented a TAC of $-1{,}329 \times 10^7$ \$.year^{-1} and an energy efficiency of 56.12%, suggesting that cheaper electricity, in order to reduce the cost of hydrogen production, may have a great positive impact on the energy efficiency of sugarcane biorefineries, due to the increase in biofuel production, as well as on their economic viability. In Case 5, for DME to be produced, it was necessary for the biorefinery to also produce methanol. In this sense, the bagasse gasification unit was activated, acting both in the production of methanol and in the supply of heat for other processes, justifying the increase in the biorefinery's payback. It is also possible to observe an increase in the energy efficiency of the biorefinery, when compared to case 3, indicating that the conversion of methanol into DME has a greater efficiency than gasification. In the same way as in case 3, as all bagasse is destined for the gasification process, the biorefinery has a system of photovoltaic panels to generate the electricity consumed. Of the evaluated cases, the one with the lowest payback value was ethanol production. Despite this, methanol production proved to be the most advantageous because of its lower TAC. Regarding the energy aspect, in the cases where energy integration was carried out, much greater energy efficiency was achieved, given that in these cases, bagasse was no longer used as a fuel to supply energy, but instead began to be used to produce biofuel.

Table 2 – Main results obtained for the evaluated cases.

Parameter	**Case 1**	**Case 2**	**Case 3**	**Case 4**	**Case 5**
TAC [$/year]	$-7{,}197 \times 10^7$	$-7{,}230 \times 10^7$	$-7{,}357 \times 10^7$	6.503×10^7	$-7{,}224 \times 10^7$
Payback [year]	3,25	3,37	4,27	-18,26	4,42
Energy Efficiency	39,5%	42,5%	66,7%	56,12%	67,5%

Conclusions

The aim of this work was to present a superstructure formulation for optimising biorefineries, capable of selecting and adjusting the scale of processes, simultaneously selecting utilities, and integrating energy between cascades. With the realisation of the cases, the effectiveness of the presented formulation was verified. In addition, it was possible to verify that of the routes evaluated, the one with the lowest PayBack was the production of ethanol by the distillery, but the one that proved to be most advantageous was the production of methanol by gasification of bagasse, as it had the lowest TAC. The results obtained show that methanol production via the CCH route is not feasible and that this is related to the high costs of producing H_2, thus suggesting that reducing these costs could have a positive impact on the energy efficiency of the biorefinery. It was also possible to verify the positive impact of energy integration between cascades in the biorefinery, both in economic and energy terms.

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References

[1] B. Linnhoff and V. Sahdev, "Pinch technology," *Ullmann's Encyclopedia of Industrial Chemistry*, 2000.
[2] A. D. Celebi, A. V. Ensinas, S. Sharma, and F. Maréchal, "Early-stage decision making approach for the selection of optimally integrated biorefinery processes," *Energy*, vol. 137, pp. 908–916, 2017, doi: 10.1016/j.energy.2017.03.080.
[3] L. Tock, M. Gassner, and F. Maréchal, "Thermochemical production of liquid fuels from biomass: Thermo-economic modeling, process design and process integration analysis," *Biomass Bioenergy*, vol. 34, no. 12, pp. 1838–1854, 2010, doi: 10.1016/j.biombioe.2010.07.018.
[4] I. Kantor, J. L. Robineau, H. Bütün, and F. Maréchal, "A Mixed-Integer Linear Programming Formulation for Optimizing Multi-Scale Material and Energy Integration," *Front Energy Res*, vol. 8, no. April, 2020, doi: 10.3389/fenrg.2020.00049.
[5] M. Bagajewicz and H. Rodera, "Energy savings in the total site heat integration across many plants," *Comput Chem Eng*, vol. 24, no. 2–7, pp. 1237–1242, Jul. 2000, doi: 10.1016/S0098-1354(00)00318-5.
[6] J. Q. Albarelli, "Produção de açúcar e etanol de primeira e segunda geração: simulação, integração energética e análise econômica," Universidade Estadual de Campinas, 2013.
[7] L. T. Fuess, M. M. de Araújo Júnior, M. L. Garcia, and M. Zaiat, "Designing full-scale biodigestion plants for the treatment of vinasse in sugarcane biorefineries: How phase separation and alkalinization impact biogas and electricity production costs?," *Chemical Engineering Research and Design*, vol. 119, pp. 209–220, 2017, doi: 10.1016/J.CHERD.2017.01.023.
[8] E. C. D. Tan *et al.*, "Process Design and Economics for the Conversion of Lignocellulosic Biomass to Hydrocarbons via Indirect Liquefaction: Thermochemical Research Pathway to High-Octane Gasoline Blendstock Through Methanol/Dimethyl Ether Intermediates," 2015. Accessed: Aug. 29, 2022. [Online]. Available: https://www.nrel.gov/docs/fy15osti/62402.pdf
[9] F. Lonis, V. Tola, and G. Cau, "Assessment of integrated energy systems for the production and use of renewable methanol by water electrolysis and CO2 hydrogenation," *Fuel*, vol. 285, p. 119160, Feb. 2021, doi: 10.1016/J.FUEL.2020.119160.
[10] Y. Khojasteh-Salkuyeh, O. Ashrafi, E. Mostafavi, and P. Navarri, "CO2utilization for methanol production; Part I: Process design and life cycle GHG assessment of different pathways," *Journal of CO2 Utilization*, vol. 50, Aug. 2021, doi: 10.1016/J.JCOU.2021.101608.