In-silico production of bioactive enrichment soil fertilizer from agricultural by-products towards bioeconomics perspectives

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ABSTRACT

Objective: To evaluate production facilities biorefinery design of bioactive enrichment soil fertilizer using food waste generated by farms in Baja California Sur (BCS), México, of five agricultural commodities towards bioeconomic perspectives.

Design/methodology/approach: BCS state was the study area. A mathematical model biorefinery design was made using a Mixed Integer Linear Program approach. Four layers of decision were used, Biomass, Production facilities, Storage and Consumer location. SuperPro Designer was used to biorefinery design and model was formulated in Phyton.

Results: Model shows two optimal production facilities: Valle de Vizcaino (VV) and Valle de Santo Domingo (VSD). VV processes strawberry and tomato with net profit of 50.28. While VSD processes orange and asparagus with net profit of 35.48. Production line goes from May to April. Ascorbic acid and quercetin were considered to enrichment the soil fertilizer.

Limitations on study/implications: This study did not produce bioactive compounds in industrial way only use mathematical modeling program and equations to predict the optimal scenario to production facilities location in an agricultural region.

Findings/conclusions: Model showed the importance of consider four interconnected decision layers. The framework was developed for capturing food waste generation dynamics. These dynamics display a very important role in all other dimensions' decisions and that an efficient biorefinery design must account for these dynamics.

Keywords: Agri-food, Biorefinery design, Food waste, bioeconomics, bioactive compounds.

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INTRODUCTION

Environmental, economic, and societal pressures necessitate a transition from linear "take-make-dispose" models of consumption and production to value networks and business models aligned with circular economy principles [1]. The so-called circular economy framework is the system in which the consumption of materials and waste generation are minimized while also recycling and reusing the residues to produce new materials [2].

In this way, the concept of turning waste into a resource is especially interesting in terms of sustainability.

Agri-food industries (AFI) generate high amounts of processing waste [3]. Some well-established applications of these wastes include their use as animal feed or soil fertilizers [4-5]. However, these AFI by-products are remarkable rich in wide range of high added-value bioactive components, such as polyphenolic compounds [6]. Polyphenols are a vast group of secondary plant metabolites that comprise thousands of compounds [7]. Polyphenols are scavengers of free radicals, which are harmful products of aerobic metabolism leading to oxidative stress in the organism [7]. Multiple *in-vitro*, *in-vivo*, and epidemiological studies have shown that polyphenols are of great interest in the prophylaxis and treatment of cardiovascular and neurological diseases, cancer, and aging-related disorders, mainly due to their remarkable antioxidant activity [8-9].

Bioactive phenolic acids and flavonoids are on the top of the well-known value pyramid of biomass, which makes AFI waste very attractive from circular bioeconomy approach, which great prospects in the pharmaceutical, cosmetics, and food industries [10]. In this context, recovering natural polyphenols from AFI waste is an excellent option, in line with the United Nations Sustainable Development Goals [11]. The overall strategy is even more remarkable when green technologies are applied, with the design of processes aiming to eliminate, or at least reduce significantly, the use and generation of hazardous substances and prevent environmental and health impacts [12]. In this scenario, the extraction, characterization, and purification of phenolic acids and polyphenols stir up an increasing scientific and commercial interest [10].

Biorefining consists of biomass exploitation to produce chemicals and energy and emerges as a potential alternative for more sustainable industrial models [13]. Nonetheless, the abundance of biomass sources, conversion technologies, and potential target-products makes the efficient design of biorefinerías a very complex task [14].

Mathematical programming has been extensively employed to facilitate this task [15, 16]. Frameworks to choose optimal technological pathway for converting a set of feed-stocks into a set of desired chemical represent important tools for deciding technological aspects of the biorefinery design [17]. However, they do not incorporate location-specific information into the decision-making process [18]. As biomass physic-chemical properties and availability are highly dependent on geography [19], this location-specific information should also be considered in the decision making-process, which should account not only for conversion technologies but for the whole biorefinery supply chain.

Biomass supply chain aspects were incorporated into a mathematical programming framework [20]. They proposed a framework for designing biomass-based energy systems that explicitly decides on cultivation, harvesting, and the centralization/decentralization of processing facilities. However, the framework applies only to a local level as it does not consider the possibility of integrating supply and demand from different regions.

From the above mentioned, the present study aims to assess the *in-silico* biorefinery design for bioactive and biofertilizer production from agricultural residues of AFI along five perishable vegetable species (commodities) supply chains in Baja California Sur, México. By using data collected at the harvest level, we examine the process towards bioeconomic perspectives.

MATERIALS AND METHODS

This study was conducted with data collected in Baja California Sur State (BCS), in five municipalities (Figure 1). FLW data of every commodity was assessed in harvest stage of supply.

Framework and mathematical model

The framework consists of two steps: (i) Model formulation and solution, and (ii) Results and evaluation. Model formulation and solution aims at instantiation the mathematical model with the data of [21] and at retrieving the instance's optimal solution. Optimal solution was drawn, as it shows in Figure 2.

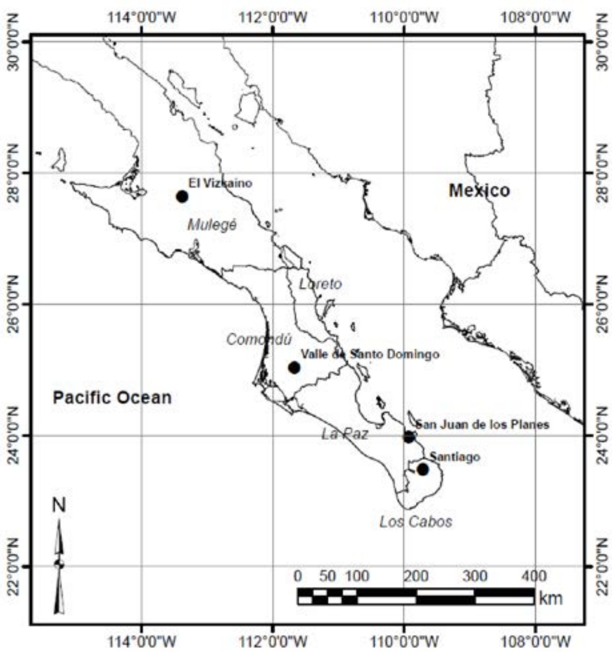

Figure 1. Map of Baja California Sur indicating the municipalities and localities included in the study. (Source Martinez-Camacho *et al.*, 2024).

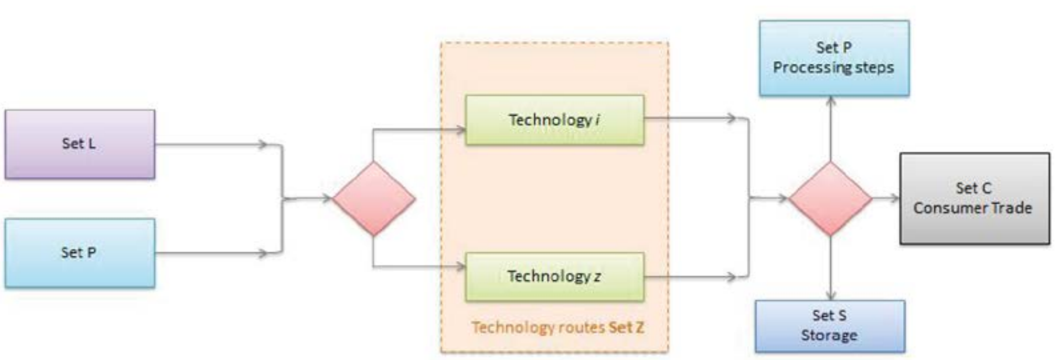

Figure 2. Mass Flow within Production Layer P. Demand is translated to a chemical species flow according to a biomass composition parameter and summed over all units. The species flows coming from sums up to those transferred from other production facilities and are split into the conversion technologies z.

The mathematical model proposed for the framework consists of a Mixed Integer Linear Program that interconnects four layers of decision (Figure 2). Each layer is represented by a set of n possible instances: Set L (Biomass cultivation locations); Set P (Possible Production facilities location); Set S (storage locations); and Set C (Possible Consumer location). The interconnections flows are referenced with a subscript q (or b) indicating a chemical species q from the Set Q (or a biomass b from Set B) and a subscript t is indicating a period from the Set T. All variable data is shown in Table 1.

The flow of biomass b transferred to the production facilities is converted to a flow of a chemical species q of the Set Q $\left(FFP_{p,q,t}\right)$ according to a composition parameter defined for each biomass b at each harvest location $f\left(X_{f,b,q}\right)$ (Eq. 1). The mass balances for the production, storage and consumer layers are developed in function of the chemical species flow.

$$FFP_{p,q,t} = \sum_{f€F} \sum_{b€B} X_{f,b,q} F^{demand} F_{f,p,b,t} \forall \left(p€P, q€Q, t€T\right) \qquad \text{(Eq. 1)}$$

The demand of biomass from all the production facilities is summed into the demand of harvested biomass at each harvest location $\left(FF^{harvested}{}_{f,b,t}\right)$ (Eq. 2).

$$FF^{harvested}{}_{f,q,t} = \sum_{p€P} F^{demand} F_{f,p,b,t} \forall \left(f€F, b€B, t€T\right) \qquad \text{(Eq. 2)}$$

The harvested biomass is transferred to the production layer for conversion. The amount of chemical q that is fed to the production facility p may be split into the z technologies available within the Set Z. The chemical species qprod produced by a technology z can have several destinations. These flows are subjected to a mass balance for each species q at each production facility p for each period t.

Table 1. Mathemathical model Data. Supplemented data to *in-silico* model for biorefinery design.

Set	Location	Set	Species		Time
			Chemical	Biomass	
Set L	Valle de Vizcaíno, Valle de Santo Domingo, Los Planes, Santiago, Todos Santos.	Set Q	Ascorbic acid, quercetin		
Set P	Valle de Vizcaíno, Zona Ejidal, Loreto, Ciudad Constitución, Ciudad Insurgentes, La Paz, Los Planes, Santiago, Todos Santos.	Set B		Asparagus, Mango, Orange, Strawberry, Tomato.	
Set S	Valle de Vizcaíno, Loreto, Ciudad Constitución, La Paz, Todos Santos	Set T			May to April, monthly assessment
Set C	Valle de Vizcaíno, Loreto, Valle de Santo Domingo, La Paz, Cabo San Lucas, San José del Cabo, Todos Santos				

This model does not need to have predefined sequential processing steps. Instead, it assumes a parallel processing network where the output of any technology may serve as input for any other technology. Each technology has its own conversion parameters defined for each pair of chemical on Set Q. When converting chemical q to qprod it is also possible to produce utilities as a co-product. Some utilities are also needed for enabling a given conversion. The utilities that are produced by a technology z can be used by another technology z' within the same production facility. The surplus (or lack) of any utility produced (or demanded) can be sold within the same production facility.

Production operational and capital costs are estimated as a function of the chemical species flow fed to each technology. The capacity of each technology on each production facility is taken as the maximum chemical species flow within this facility on all operational periods.

Storage facilities are considered for implementing minimal storage policies and transport modal shifts. For instance, it may be defined a port location on Set S that receives some material by road transport (from production to storage facilities).

The objective function is defined as the Net Present Values (NPV) of the cash flow generated by the operation. Production and Storage Investments are incidents in the first period of operation. Profit is incident in the middle of each period and is discounted to present value by an interest rate.

Case of study

The framework presented in section above is illustrated through a case study on the in silico production of biofertilizer and enrichment bioactive compound serum produced via fermentation of five commodities waste. The potential locations for the operation implementation are all in BCS state (Harvest, production and storage), but trade steps could be worldwide.

The biomass cultivation layer is segmented according to agricultural municipalities inside BCS state (Figure 1). The strawberry, mango, tomato, asparagus and orange planted land are taken according to official data from SIAP database [22]. The commodities species selected for the model are the most productive in BCS state. The productivity data and planting, maintenance, and harvesting costs were taken from [21] and they were also used for estimation.

The Set P with all possible production facilities location was defined as the union of agricultural region point and distributor market location sets. This enables production facilities to be close to the biomass supply. The production facilities design allows producing biofertilizer and bioactive compound serum, with the possibility to recirculate used water. The only technology considered for producing serum in the model is the fermentation/extraction process. The process consists on several operations grouped in four: (i) commodity preparation, responsible for the transport and processing of raw waste, washing, cutting and selection; (ii) inoculum preparation, responsible for the processing of microorganism for fermentation; (iii) fermentation/extraction, responsible for mixing and fermentation parameters; (iv) separation, responsible of centrifugation, drying stage and packing operations. A water recovery stage was design after primary washing. A water evaporator was considered to burn residual water. A visual summary was made with SuperPro Designer of all technologies considered as is shown in Figure 3.

RESULTS AND DISCUSSION

The mathematical model shows two optimal production facilities in two different locations: Valle de Vizcaino (VV) and Valle de Santo Domingo (VSD). Figure 4 shows the NPV breakdown for the two optimal solutions for the operation and return rate smaller than 2 years in which chemical logistics and production/operation costs are the major negative contributors. The total investment on the operation is paid back during the 3rd year of operation, already considering the 1.5 years construction period.

The revenues reported in Figure 4 are already net of taxes. Thus, the overall effect of taxes on the operation's feasibility is not shown in the waterfall. The operation revenue comes exclusively from chemical sales. The only chemicals produced were ascorbic acid, quercetin and biofertilizer. Other organic acids are not considered because the purification process increases the operation cost that affects net profit in significant way [23]. Energy had presented a diminished relevance for the operations NPV. However, it is important to notice that only a single type of recirculation process is considered. Water recirculation is crucial to allow the continuity of the overall process because de production facilities are located in desert and extreme weather region [24]. Figure 4 also shows how important raw material costs are to the operations NPV. In this case of study, chemicals are completely dependent of raw material available state, so the raw material transportation was taken as opened dump tank [25].

Valle de Santo Domingo is a very competitive and well-positioned spot for production [22]. It presents high productive harvest lands availability [22]. Also, its routes to reach production facilities are near to [18]. VSD facilities process orange and asparagus waste

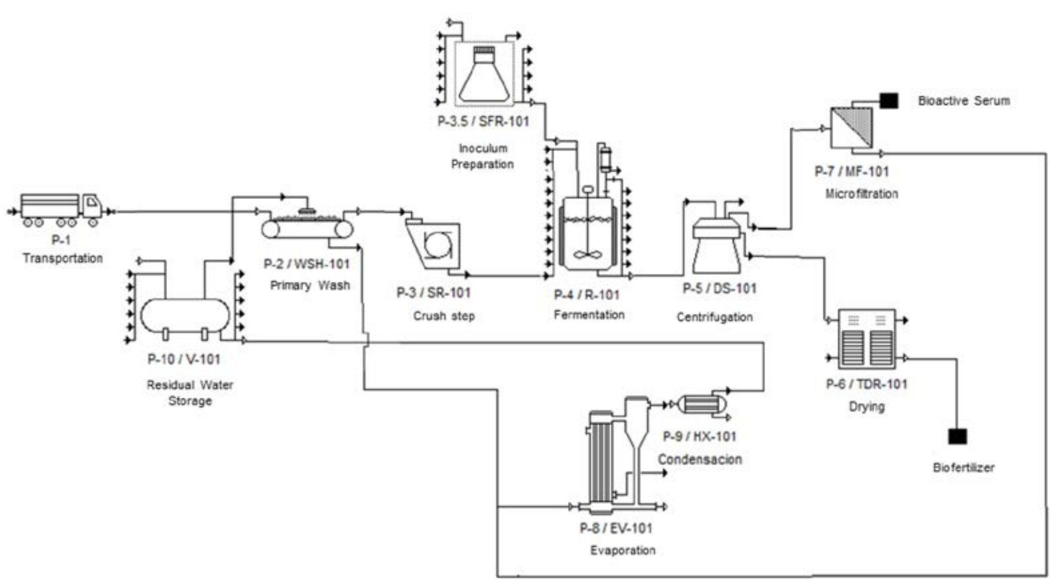

Figure 3. Visual representation of technologies and steps considered. Equipment was represented as visual symbol.

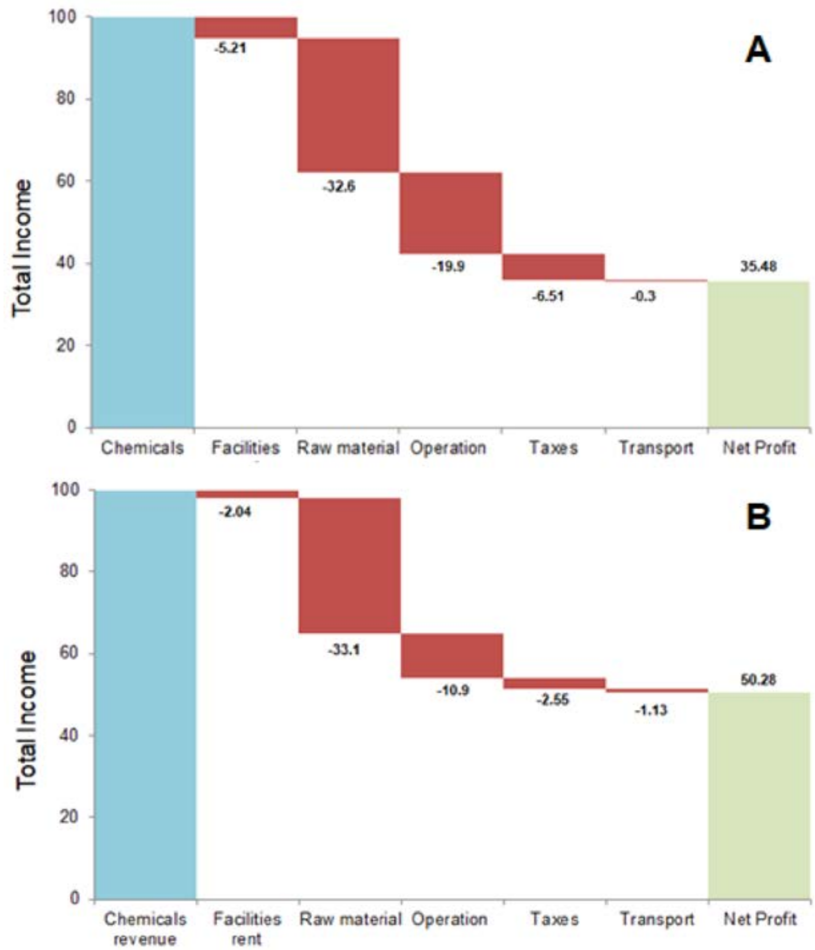

Figure 4: Breakdown of the operations Net Present Value. Revenues are already net of sales taxes. A) Valle de Vizcaino scene; B) Valle de Santo Domingo scene.

in a timeline going from May to April ensuring a complete production year. Harvest scheduling is intimately related to food waste generation, which is one of the most critical parameters for biorefinery modeling [26]. This scheme is only feasible with the assumption that the simple transference of raw material between locations of the same owner (no sale transaction involved) is free of taxes [27].

Productivity affects several aspects of operations dynamics, especially the amount of harvested land needed to buy raw material. Also, the extra land needed may push the operations to collect biomass on further distances, as the extra land required may not be available on the limits of production facilities. This extra distance might under hinder the operations performance and are not fully captured in the present model.

CONCLUSIONS

A mathematical programming framework was presented for assessing the optimal design of biorefineries considering four interconnected decision layers: Biomass, Technology, Operation, and Consumers. The framework was illustrated through a case study on bioactive compound enrichment that may use water recirculation. The framework was developed for capturing food waste generation dynamics. It was shown that theses dynamics display a very important role in all other dimensions' decisions and that an efficient biorefinery design must account for these dynamics. Finally, the technological aspects of the biorefinery were able to be captured within the parallel processing representation proposed in the present work. This representation has the advantage of supporting the addition of new process technologies to the model with little effort even if it has several interconnections to other existing technologies.

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