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A Multiobjective Optimization Approach for the Development of a Sustainable Supply Chain of a New Fixative in the Perfume Industry

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ABSTRACT: *Ambrox* is an important fixative used in the manufacture of perfumes. It is obtained through complex chemical synthesis routes with high costs. Recent research efforts at the Institute of Chemical and Biological Researches at the Universidad Michoacana have led to the one-step synthesis of *Ambrox* from extracts of *Ageratina jocotepecana* (an endemic plant of the State of Michoacán in Mexico). This new chemical route is attractive from a manufacturing perspective. However, there are several challenges for the industrial application of this plant and its incorporation in the supply chain of the perfume industry. This paper presents a multiobjective optimization approach for the development and assessment of the supply chain of *Ageratina jocotepecana* to account for its growth in current and reclaimed lands, distribution, processing to yield *Ambrox*, and distribution of products. The approach accounts for the economic, environmental, and social aspects and establishes systematic trade-offs. A case study is solved to consider the supply chain and the trade-offs of the multiple objectives.

KEYWORDS: *Ambrox, Ageratina jocotepecana, Perfume industry, Optimization, Supply chain*

INTRODUCTION

The three main components of a perfume are fragrant oils, fixatives, and solvents. A fixative is a material with low volatility that provides the long-term scent, aides in mixing with the other materials, and extends the shelf life of the perfume. The fixatives are typically expensive ingredients of the perfume.[1] A commonly used fixative is *Ambergris*, which is a waxy material produced in the digestive systems of certain whale species (*Physeter macrocephalus*). Because of the limited supply of Ambergris and its relatively high cost, synthetic alternatives have been considered. A particularly effective synthetic fixative substitute, is *Ambrox* ((−)-8α-12-dihydroxy-13,14,15,16-tetranorlabdane).[2,3] The chemical structure is shown in Figure 1.

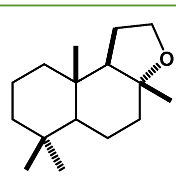

Figure 1. Chemical structure of *Ambrox*.

All the chemical routes reported to synthesize *Ambrox* involve several chemical steps having high processing costs, long reaction times, and severe processing conditions such as high pressure and temperature.[1,4−7] These routes pose challenges for profitability and manufacturing safety. Recently, *Ageratina jocotepecana*, an endemic plant of the State of Michoacán in Mexico, has been characterized to contain labdane diterpenes that are precursors of *Ambrox*.[8] Furthermore, *A. jocotepecana* extracts also contain (−)-8α-12- dihydroxy-13,14,15,16-tetranorlabdane, which is a direct precursor for the synthesis of *Ambrox* because it requires only one reaction (chemical cyclization) to obtain *Ambrox* (Figure 2).[9]

The preparation of *Ambrox* by the chemical cyclization of (−)-8α-12-dihydroxy-13,14,15,16-tetranorlabdane obtained from the stems of *A. jocotepecana* offers several advantages over current chemical synthesis routes, reducing the synthesis to only one step under mild conditions and high conversion rates. Thus, it is important to determine, at least preliminary, if it has

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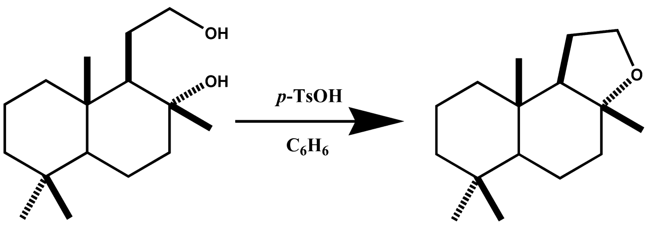

Figure 2. Chemical cyclization to obtain *Ambrox* from (−)-8α-12-dihydroxy-13,14,15,16-tetranorlabdane.

the potential to be exploited as an industrial process in the State of Michoacán in México. To accomplish this, the optimization of the supply chain (SC) has to be performed. The optimization of the SC will help maximize the profit of the global process, while reducing the environmental impact. The environmental impact will be assessed through Eco-indicator 99, which is obtained with the life cycle assessment (LCA) of the process. This way, it can be determined if the industrial production of *Ambrox* from *A. jocotepecana* is sustainable from economic, environmental, and social points of view.

A supply chain is defined as "a network of facilities and distribution mechanisms that perform the functions of material procurement, material transformation to intermediates and final products, and distribution of these products to customers".[10] Several models and studies have been developed for the SCs associated with the petrochemical industry.[11−15] These models have been extended to the optimization of the SCs associated with biorefineries, where the selection of feedstocks, products, processing routes, location of processing facilities, storage, and transportation are simultaneously evaluated and optimized.[16−23] The optimization of the SCs associated with biorefineries entails addressing various challenges such as considering the entire environmental impact involved,[24] social benefit obtained,[25] and safety issues.[26]

The SC associated with *Ambrox* production from *A. jocotepecana* involves unique features and challenges. For instance, *A. jocotepecana* only grows in a specific region of the State of Michoacán, Mexico. The largest potential consumers (the perfume industry) are located primarily in Europe. The economic, environmental, and social factors involved in the introduction of *A. jocotepecana* into the perfume supply chain must be considered. Therefore, in this paper, a mathematical model for the SC optimization associated with *A. jocotepecana* to obtain *Ambrox* is presented. A multiobjective optimization approach is developed to account for the economic, environmental, and social issues of the targeted supply chain.

■ PROBLEM STATEMENT

It is desired to assess the introduction of *Ageratina jocotepecana* into the perfume SC through conversion to *Ambrox* and to assess the economic, environmental, and social implications. Therefore, the problem addressed in this paper consists of determining the best options to install processing facilities for (−)-8α-12-dihydroxy-13,14,15,16-tetranorlabdane extraction and *Ambrox* production and distribution. Figure 3 shows a superstructure that represents all the required steps for *Ambrox* production from *A. jocotepecana* in Michoacán, Mexico. Focus is given to three main components of the SC: (1) harvesting sites for *Ageratina jocotepecana* production, (2) processing plants for the synthesis of *Ambrox*, and (3) markets for the final products and subproducts.

The problem consists in defining the location and cultivation area of *A. jocotepecana* and the existence, location, and capacity of processing facilities required to satisfy specific demands in the final markets, while maximizing the profit and social benefits and reducing the environmental impact. For this purpose, a modeling framework that includes all the steps and alternatives from raw materials to final products related to the supply chain has been developed.

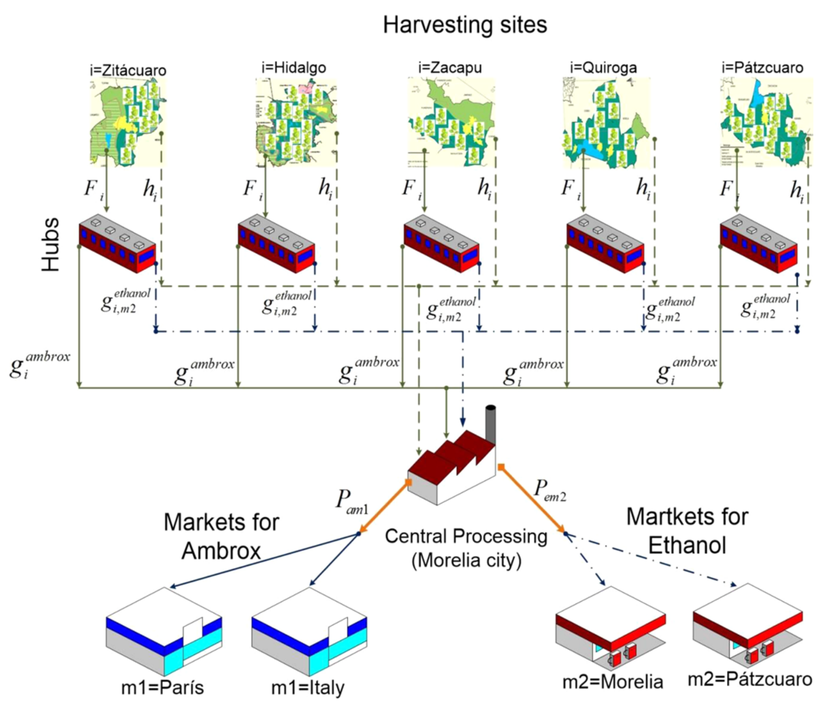

Figure 3. Proposed superstructure for the supply chain of *Ambrox* production from *Ageratina jocotepecana*.

Table 1. Potential Use of Land for *Ageratina jocotepecana* Growth in Each Municipality[29]

	area (ha)			
municipality	farming	current area with *Ageratina jocotepecana*	urban zone	total
Hidalgo	153,921.9	6	24,158.15	1,118,522.35
Pátzcuaro	182,621.6	2	19,519.34	419,973.15
Quiroga	84,450.9	1	6,860.92	204,095.47
Zacapu	180,221.0	2	21,156.97	430,055.32
Zitácuaro	209,709.2	2	27,733.56	482,077.73

■ SUPPLY CHAIN OPTIMIZATION

First, for the feedstock cultivation, it is necessary to consider the type of soil and climate conditions that allow the development of the *Ageratina jocotepecana* crops. The plant was endemically found along the road Morelia-Zacapu, which has mild weather with andosol soil. For these reasons, municipalities such as Quiroga, Pátzcuaro, Zacapu, Zitácuaro, and Hidalgo (that have similar weather and soil conditions) are considered potential harvesting sites for *A. jocotepecana*. These municipalities are located in the State of Michoacán in Mexico. The data for the current distribution of land according to its use in each municipality is shown in Table 1. It is assumed that only the farming area can be used for *A. jocotepecana* production (to avoid the environmental impact for the land change of use).

To determine the total extension of land used to cultivate *A. jocotepecana* in each municipality (A_i), a balance considering the area currently occupied by *A. jocotepecana* (A_i^{existing}) and the new area required (A_i^{new}) is used

$$A_i = A_i^{\text{existing}} + A_i^{\text{new}}, \quad \forall\ i \in I \tag{1}$$

The cultivated area has to be lower than the total available area. A maximum limit for the area in each municipality is defined to avoid excessive change of land or even change of crops. This can be done with the following constraint

$$A_i \le A_i^{\max}, \quad \forall\ i \in I \tag{2}$$

The maximum area cultivated with *A. jocotepecana* ($A_i^{\max}$) can be defined in the fraction of the total available area in each municipality.

The amount of stems of *A. jocotepecana* per hectare is proportional to the cultivated area and the yield factor (α_i) (Table 2), which can be obtained from field data

$$F_i = \alpha_i A_i, \quad \forall\ i \in I \tag{3}$$

Table 2. Production Yield of Bioethanol and *Ambrox* from *Ageratina jocotepecana*[9,35−37]

municipality	bioethanol (β_i^{ethnaol})	*Ambrox* (β_i^{Ambrox})	*Ageratina jocotepecana* (ton/ha) (α_i)
Hidalgo	0.65	5.31×10^{-04}	13
Pátzcuaro	0.6	6.31×10^{-04}	17
Quiroga	0.59	5.21×10^{-04}	20
Zacapu	0.55	5.65×10^{-04}	15
Zitácuaro	0.65	5.66×10^{-04}	10

The balance for the stems of *A. jocotepecana* indicates that the total flow of stems is equal to the stems sent to the preprocessing plants plus the stems sent to the central plant from the harvesting site *i*.

$$F_i \ge f_i + h_i, \quad \forall\ i \in I \tag{4}$$

It is shown that the preprocessing plants can receive stems only from the harvesting site associated with their location. On the other hand, the central processing plant can receive stems from any harvesting site, and thus, the total flow in the central plant is equal to the sum of all the flows sent from the different municipalities.

$$F_{\text{central}} = \sum_i h_i \tag{5}$$

In the model formulation, it is considered that the main product is *Ambrox* and that the remaining biomass can be used to produce bioethanol as a subproduct with commercial value. In the preprocessing plants, the *Ambrox* and bioethanol produced are functions of the stems processed and the yield factors to *Ambrox* and bioethanol production shown in Table 2.

Therefore, the production of *Ambrox* and bioethanol in preprocessing plants can be described by eqs 6 and 7 and in the central plant by eqs 8 and 9. These equations imply that the production in a given plant is a function of the flow of stems times the yield factor for a specific product.

$$g_i^{Ambrox} = f_i \beta_i^{Ambrox}, \quad \forall\ i \in I \tag{6}$$

$$g_i^{\text{ethanol}} = f_i \beta_i^{\text{ethanol}}, \quad \forall\ i \in I \tag{7}$$

$$P^{Ambrox} = F_{\text{central}} \gamma^{Ambrox} \tag{8}$$

$$P^{\text{ethanol}} = F_{\text{central}} \gamma^{\text{ethanol}} \tag{9}$$

This way, the total *Ambrox* and bioethanol produced are the sum of the production in the preprocessing and central plants as follows

$$M^{Ambrox} = P^{Ambrox} + \sum_i g_i^{Ambrox} \tag{10}$$

$$M^{\text{ethanol}} = P^{\text{ethanol}} + \sum_i g_i^{\text{ethanol}} \tag{11}$$

The products must be distributed to the markets as follows

$$M^{Ambrox} = \sum_{\text{m1}} S_{\text{m1}}^{Ambrox} \tag{12}$$

$$M^{\text{ethanol}} = \sum_{\text{m2}} S_{\text{m2}}^{\text{ethanol}} \tag{13}$$

A constraint for the demands in the markets must be included. This implies that the total *Ambrox* and bioethanol produced must be lower than or equal to the demand in each market (otherwise there is not a market for the excess product).

$$S_{\text{m1}}^{Ambrox} \le P_{\text{m1}}^{\max Ambrox}, \quad \forall\ \text{m1} \in M1 \tag{14}$$

$$S_{\text{m2}}^{\text{ethanol}} \le P_{\text{m2}}^{\max\ \text{ethanol}}, \quad \forall\ \text{m2} \in M2 \tag{15}$$

It should be noted that the amount of bioethanol produced from *A. jocotepecana* is not very significant. This is mainly limited by the demand of *Ambrox*. In order to satisfy the total demand of *Ambrox*, the amount of biomass produced is relatively small, and thus, not much bioethanol can be produced. The main assumption here is that there is a yield factor from the stems of *A. jocotepecana* to bioethanol and that this factor was obtained experimentally. The idea to produce bioethanol from the wasted biomass is to obtain additional benefits (economic and environmental) from the entire process.

The total cost of the process is represented by eq 16, which considers the cost of the raw material production, raw material transportation, fixed and variable costs of processing in the preprocessing and central plants, and transportation costs of the final products to the markets.

$$\begin{aligned} \text{cost} = & \sum_i C_i^{\text{harvest}} F_i + \sum_i C_{\text{prepropla},i}^{\text{capprocess}} + \sum C_{\text{central}}^{\text{capprocess}} \\ & + \sum_i C_i^{\text{trans}-Ambrox} g_i^{Ambrox} \\ & + \sum_{\text{m2}} \sum_i C_{i,\text{m2}}^{\text{transpo}-\text{ethanol}} g_{i,\text{m2}}^{\text{ethanol}} + \sum_i C_i^{\text{transpo}-\text{plant}} h_i \\ & + \sum_{\text{m1}} C_{\text{m1}}^{\text{transpo}-Ambrox} P_{\text{m1}}^{Ambrox} \\ & + \sum_{\text{m2}} P_{\text{m2}}^{\text{ethanol}} C_{\text{m2}}^{\text{transpo}-\text{ethanol}} \end{aligned} \tag{16}$$

The transportation of the raw materials and products depends on the location of the harvesting sites and preprocessing plants. Table 3 shows the associated costs for this activity, and these are calculated taking into consideration the distance between the source and destination of the materials.

Table 3. Transportation Costs of Raw Material, Products, and Byproducts[29,30]

municipality	distance (km) to the central plant	transport of bioethanol ($/gallon)	transport of raw materials and products (*Ambrox*) ($/ton)
Hidalgo	103	0.00943	3.16
Pátzcuaro	56.4	0.00516	1.73
Quiroga	42	0.00384	1.28
Zacapu	82	0.00750	2.51
Zitácuaro	152	0.01390	4.66

The unit costs for the preprocessing and central plants used in eq 16 depend on the processing capacity. However, due to the fact that the capacity of the plant is an optimization variable, this is handled with two disjunctions. The first disjunction is used to determine the location, capacity, and number of required preprocessing plants

$$\bigvee_p \begin{bmatrix} Y_{p,i} \\ F_{Aj,i,p}^{\text{lower}} \le F_{Aj,i} \le F_{Aj,i,p}^{\text{upper}} \\ C_{\text{prepropla},i}^{\text{capprocess}} = C_{i,p}^{\text{F}} + C_{i,p}^{\text{V}} F_{Aj,i} \end{bmatrix}, \quad \forall\, i \in I$$

If the Boolean variable is true, then a given capacity for the plant will be selected, and the appropriate costs will be added. The disjunction is reformulated as a set of algebraic equations as follows. First, only one section must be selected (the first section corresponds to a capacity of zero, and the unit costs are zero)

$$\sum_p y_{p,i} = 1, \quad \forall\, i \tag{17}$$

Then, the continuous variables are disaggregated

$$F_{Aj,i} = \sum_p \text{DF}_{Aj,i,p}, \quad \forall\, i \tag{18}$$

$$C_{\text{prepropla},i}^{\text{capprocess}} = \sum_p \text{DC}_{i,p}^{\text{Cap}}, \quad \forall\, i \tag{19}$$

The relationships are stated in terms of the disaggregated variables

$$y_{p,i} F_{Aj,i,p}^{\text{lower}} \le \text{DF}_{Aj,i,p} \le y_{p,i} F_{Aj,i,p}^{\text{upper}}, \quad \forall\, p, \forall\, i \tag{20}$$

$$\text{DC}_{i,p}^{\text{Cap}} = C_{i,p}^{\text{F}} y_{p,i} + C_{i,p}^{\text{V}} \text{DF}_{Aj,i}, \quad \forall\, \text{p}, \forall\, i \tag{21}$$

It should be noted that eq 21 includes a binary variable ($y_{p,i}$), which is multiplied by the unit fixed cost, and only if the binary variable is equal to one will the cost will be included. The variable part is a function of the disaggregated flow that can be zero, and thus, the cost will only be included if the binary variable is equal to one in a segment where the flows can be greater than zero.

In a similar way, a second disjunction is used to determine the existence or not of the central processing plant. In this case, the location is not a decision variable, and only the capacity of the plant is considered.

$$\bigvee_p \begin{bmatrix} Y_p \\ F_{Aj,\text{central,p}}^{\text{lower}} \le F_{\text{central}} \le F_{Aj,\text{central,p}}^{\text{upper}} \\ C_{\text{central}}^{\text{capprocess}} = C_{\text{cen,p}}^{\text{F}} + C_{\text{cen,p}}^{\text{V}} F_{\text{central}} \end{bmatrix}$$

The disjunction is again reformulated as a set of algebraic constraints as follows

$$\sum_p y_{\text{cen,p}} = 1 \tag{22}$$

$$F_{\text{central}} = \sum_p \text{DF}_{Aj,\text{cen,p}} \tag{23}$$

$$C_{\text{central}}^{\text{capprocess}} = \sum_p \text{DC}_{\text{cen,p}}^{\text{Cap}} \tag{24}$$

$$y_{\text{cen,p}} F_{Aj,\text{central,p}}^{\text{lower}} \le \text{DF}_{Aj,\text{cen,p}} \le y_{\text{cen,p}} F_{Aj,\text{central,p}}^{\text{upper}}, \quad \forall\, \text{p} \tag{25}$$

$$\text{DC}_{\text{cen,p}}^{\text{Cap}} = \text{C}_{\text{cen,p}}^{\text{F}} y_{\text{cen,p}} + \text{C}_{\text{cen,p}}^{\text{V}} \text{DF}_{Aj,\text{cen,p}}, \quad \forall\, p \tag{26}$$

The selection between a central or preprocessing plant is based on the amount of raw material that is processed, transportation cost, market demand of *Ambrox*, and processing costs taking into account the capacity of each plant. The cost of the plant can be divided in two components: variable costs (Table 4) and fixed costs (Table 5). The variable costs are the costs associated with the processing of raw materials to yield products and are given by all the activities that are required in the production process; an example calculation of the variable costs for a preprocessing plant with a capacity of 40.8 ton/day is shown in Table 6. Notice that the variable costs for the central plants are lower than the costs

Table 4. Variable Costs Associated with Processing Plants

minimum capacity (ton/day)	maximum capacity (ton/day)	central plant ($/ton)	preprocessing plant ($/ton)
0	0	0	0
0	40.8	15	20
40.8	122.4	13	17
122.4	149.6	10	15

Table 5. Fixed Costs Associated with the Processing Plants[31]

minimum capacity (ton/day)	maximum capacity (ton/day)	cost ($/y)
0	0	0
0	40.8	15000
40.8	122.4	50000
122.4	149.6	158000

Table 6. Variable Costs of Processing Plants[32]

concept	energy consumed (kWh/ton)	cost ($/ton)
transportation line	5.705	1.990
drying	18.7643	3.252
strain	5.353	2.020
filtered	3.757	2.150
manipulation	3.194	1.606
heating	1.080	2.173
evaporating	19.690	3.337
shake	3.000	2.247
pumping	0.300	1.810
total	60.843	20.585

for preprocessing plants. This is associated with the fact that the central plant is located in an industrialized zone, and all the utilities and required infrastructure are readily available. On the other hand, the fixed costs are also expressed in terms of the capacity of each plant (ton of *Ageratina jocotepecana* stems processed per day). An economic life of 10 years is considered with an interest rate of 12%.

The social aspect associated with the process is measured through the job generation. This is shown in eq 27. This equation considers the created jobs in the harvesting sites, processing plants (preprocessing and central), and required labor for transportation of raw material and final products. The details of the jobs generated for each of these activities along with the associated cost are shown in Tables 7 and 8. It is shown that

Table 7. Jobs Generation and Costs Associated with *Ageratina jocotepecana* Growing[30,33]

activity	jobs generated (jobs/ha)	cost ($/ha)[a]
cropping	0.137	994
harvesting	0.129	556
transportation	0.0004332	1.28[a]

[a]Distance for this cost is 42 km.

Table 8. Jobs Generated for *Ambrox* and Bioethanol Production[33,34]

activity	jobs/ton
processing in the preprocessing plants	0.25
transport of *Ambrox* between plants	1.00
transport of bioethanol to the central plant	1.00
processing in the central plant	0.25
transport of *Ambrox* to the markets	2.00

growing *A. jocotepecana* might have a positive social impact due to the generation of jobs. Nevertheless, it must be considered that job generation is not the only measure of the social impacts of a project. Other important aspects to consider are worker safety, risk assessment. and community economic impacts.

$$\begin{aligned} N_{\text{jobs}} = {} & \sum_i n_i^{\text{harvest}} F_i + \sum_i n_i^{\text{process}} f_i + \sum_i n_i^{\text{process}} h_i \\ & + \sum_i n_i^{\text{transpo}-Ambrox} g_i^{Ambrox} \\ & + \sum_{m2} \sum_i n_{ji,m2}^{\text{transpo}-\text{ethanol}} g_{i,m2}^{\text{ethanol}} + \sum_i n_i^{\text{transpo}-\text{plant}} h_i \\ & + \sum_{m1} n_{m1}^{\text{transpo}-Ambrox} P_{m1}^{Ambrox} \\ & + \sum_{m2} P_{m2}^{\text{ethanol}} n_{m2}^{\text{transpo}-\text{ethanol}} \end{aligned} \qquad (27)$$

The total sales of the products are calculated as the sum of the sales of each product

$$\text{Sales} = \sum_{m1} \text{Price}_{m1}^{Ambrox} S_{m1}^{Ambrox} + \sum_{m2} \text{Price}_{m2}^{\text{ethanol}} S_{m2}^{\text{ethanol}} \qquad (28)$$

This way, the net profit is equal to the sales minus the costs

$$\text{NP} = \text{sales} - \text{cost} \qquad (29)$$

Additionally, it is important to evaluate the environmental impact associated with the process to evaluate if it is environmentally sustainable. The environmental impact is evaluated through the Eco-indicator 99 based on the life cycle analysis methodology. This methodology includes the environmental impact caused by a specific substance, process, or activity necessary in a process.[27] The Eco-indicator 99 considers 11 impact categories, which are classified into three main damage categories as shown in Figure 4.

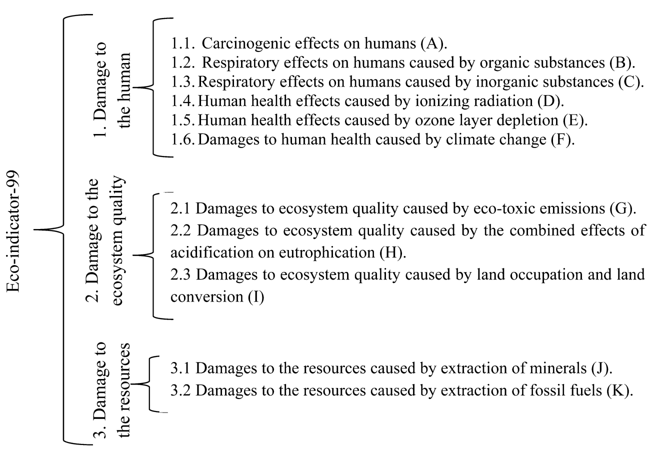

Figure 4. Eco-indicator 99 methodology.

The global environmental impact (EI) is the value that is generated for all the supply chain to carry out the process at the industrial scale. For the specific case of *Ambrox* production from *A. jocotepecana*, eq 30 applies and considers the environmental impact caused by extraction of raw material and for the production of *Ambrox* and bioethanol.

$$\text{EI}_{\text{Global}} = \text{EI}_{\text{rawmaterial}} + \text{EI}_{\text{bioethanolpro}} + \text{EI}_{Ambrox\text{pro}} \qquad (30)$$

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Table 9. Values for Damages Associated with the Cultivation of *Ageratina jocotepecana*

discharges to water	compound	emissions per ton of *A. jocotepecana*	associated EI-99 (points)	type of damage
1	PO_4^{3-}	382.1	–	–
2	NO_3^-	194	–	–
3	pesticides	45 per ha	0.000395 factor × ha × y	0.0177 G
emissions to air				
1	CO_2	192	0.00545 factor × ton emissions	1.04 F
2	NO_x	1.024	2.30, 0.445	2.3552 C, 0.455 H
3	SO_x	0.062	1.42, 0.0812	0.088 C, 0.00503H
4	N_2O	0.2	1.79	0.358 C
5	NH_3	0.0776	2.21, 1.21	0.0171 C, 0.093 H
occupation	factor × m^2 × y		0.00000749	I
conversion	factor × m^2		0.000268	I

Each of the terms in the previous equation considers the three damage factors consider in the Eco-indicator 99 methodology: damage to the human health, damage to resources, and damage to the ecosystem. The value for each damage is evaluated with the following equations

$$\mathrm{EI}_{\mathrm{rawmaterial}} = D_{\mathrm{humanhealth}}^{\mathrm{RMC}} + D_{\mathrm{resources}}^{\mathrm{RMC}} + D_{\mathrm{ecosystem}}^{\mathrm{RMC}} \tag{31}$$

$$\mathrm{EI}_{Ambrox\mathrm{pro}} = D_{\mathrm{humanhealth}}^{\mathrm{AP}} + D_{\mathrm{resources}}^{\mathrm{AP}} + D_{\mathrm{ecosystem}}^{\mathrm{AP}} \tag{32}$$

$$\mathrm{EI}_{\mathrm{bioethanolpro}} = D_{\mathrm{humanhealth}}^{\mathrm{BP}} + D_{\mathrm{resources}}^{\mathrm{BP}} + D_{\mathrm{ecosystem}}^{\mathrm{BP}} \tag{33}$$

$$\begin{aligned} D_{\mathrm{humanhealth}}^{\mathrm{RMC}} &= \sum_i D_{\mathrm{HE}}^{\mathrm{carcinogenic}} F_i + \sum_i D_{\mathrm{HE}}^{R-\mathrm{organicsubstances}} F_i \\ &+ \sum_i D_{\mathrm{HE}}^{R-\mathrm{Inorganicsubstances}} F_i + \sum_i D_{\mathrm{HE}}^{\mathrm{ionzingradiation}} F_i \\ &+ \sum_i D_{HE}^{\mathrm{ozonedepletion}} F_i + \sum_i D_{\mathrm{HE}}^{\mathrm{climatechange}} F_i, \quad \forall\ i \in I \end{aligned} \tag{34}$$

$$\begin{aligned} D_{\mathrm{ecosystem}}^{\mathrm{RMC}} &= \sum_i D_{\mathrm{EC}}^{\mathrm{ecotoxicemissions}} F_i + \sum_i D_{\mathrm{EC}}^{\mathrm{acidification}} F_i \\ &+ \sum_i D_{\mathrm{EC}}^{\mathrm{landoccupation}} A_i^{\mathrm{existing}} + \sum_i D_{\mathrm{EC}}^{\mathrm{landoccupation}} A_i^{\mathrm{new}}, \quad \forall\ i \in I \end{aligned} \tag{35}$$

$$D_{\mathrm{resources}}^{\mathrm{RMC}} = \sum_i D_{\mathrm{RE}}^{\mathrm{fossilfuels}} F_i + \sum_i D_{\mathrm{RE}}^{\mathrm{mineralextraction}} F_i, \quad \forall\ i \in I \tag{36}$$

$$\begin{aligned} D_{\mathrm{humanhealth}}^{\mathrm{AP}} &= \mathrm{AD}_{\mathrm{HE}}^{\mathrm{carcinogenic}} P^{Amrbrox} + \mathrm{AD}_{\mathrm{HE}}^{R-\mathrm{organicsubstances}} P^{Amrbrox} \\ &+ \mathrm{AD}_{\mathrm{HE}}^{R-\mathrm{inorganicsubstances}} P^{Amrbrox} \\ &+ \mathrm{AD}_{\mathrm{HE}}^{\mathrm{ionsingradation}} P^{Amrbrox} + \mathrm{AD}_{\mathrm{HE}}^{\mathrm{ozonedepletion}} P^{Amrbrox} \\ &+ \mathrm{AD}_{\mathrm{HE}}^{\mathrm{climatechange}} P^{Amrbrox} \end{aligned} \tag{37}$$

$$\begin{aligned} D_{\mathrm{ecosystem}}^{\mathrm{AP}} &= \mathrm{AD}_{\mathrm{EC}}^{\mathrm{ecotoxicemissions}} P^{Ambrox} + \mathrm{AD}_{\mathrm{EC}}^{\mathrm{acidification}} P^{Ambrox} \\ &+ \mathrm{AD}_{\mathrm{EC}}^{\mathrm{landoccupation}} \mathrm{NAVE} \end{aligned} \tag{38}$$

$$D_{\mathrm{resources}}^{\mathrm{AP}} = \mathrm{AD}_{\mathrm{RE}}^{\mathrm{fossilfuels}} P^{Ambrox} + \mathrm{AD}_{\mathrm{RE}}^{\mathrm{mineralextraction}} P^{Ambrox} \tag{39}$$

$$\begin{aligned} D_{\mathrm{humanhealth}}^{\mathrm{BP}} &= \sum_{\mathrm{m2}} \mathrm{BD}_{\mathrm{HE}}^{\mathrm{carcinogenic}} M_{\mathrm{m2}}^{\mathrm{ethanol}} \\ &+ \sum_{\mathrm{m2}} \mathrm{BD}_{\mathrm{HE}}^{R-\mathrm{organicsubstances}} M_{\mathrm{m2}\ \ i}^{\mathrm{ethanol}} \\ &+ \sum_{\mathrm{m2}} \mathrm{BD}_{\mathrm{HE}}^{R-\mathrm{inorganicsubstances}} M_{\mathrm{m2}\ \ i}^{\mathrm{ethanol}} \\ &+ \sum_{m2} \mathrm{BD}_{\mathrm{HE}}^{\mathrm{ionsingradation}} M_{\mathrm{m2}}^{\mathrm{ethanol}} \\ &+ \sum_{\mathrm{m2}} \mathrm{BD}_{\mathrm{HE}}^{\mathrm{ozonedepletion}} M_{m2}^{\mathrm{ethanol}} \\ &+ \sum_{\mathrm{m2}} \mathrm{BD}_{\mathrm{HE}}^{\mathrm{climatechange}} M_{\mathrm{m2}}^{\mathrm{ethanol}}, \quad \forall\ \mathrm{m2} \in M2 \end{aligned} \tag{40}$$

$$\begin{aligned} D_{\mathrm{ecosystem}}^{\mathrm{BP}} &= \sum_{\mathrm{m2}} \mathrm{BD}_{\mathrm{EC}}^{\mathrm{ecotoxicemissions}} M_{\mathrm{m2}}^{ethanol} \\ &+ \sum_{m2} BD_{\mathrm{EC}}^{\mathrm{acidification}} M_{\mathrm{m2}}^{\mathrm{ethanol}} \\ &+ \mathrm{BD}_{\mathrm{EC}}^{\mathrm{landoccupation}} \mathrm{NAVE}, \quad \forall\ \mathrm{m2} \in M2 \end{aligned} \tag{41}$$

$$\begin{aligned} D_{\mathrm{resources}}^{\mathrm{BP}} &= \sum_{\mathrm{m2}} \mathrm{BD}_{\mathrm{RE}}^{\mathrm{fossilfuels}} M_{m2}^{\mathrm{ethanol}} \\ &+ \sum_{\mathrm{m2}} \mathrm{BD}_{\mathrm{RE}}^{\mathrm{mineralextraction}} M_{\mathrm{m2}}^{\mathrm{ethanol}}, \quad \forall\ \mathrm{m2} \in M2 \end{aligned} \tag{42}$$

In previous relationships, AD is the damage associated with the production of *Ambrox*, BD is the damage associated with the production of bioethanol, and NAVE is the area required for the installation of the plant. The values for the considered factors are shown in Tables 9, 10, and 11. The factors were taken from Geodkoop and Spriensma.[27] The amount of emissions were estimated tanking as basis similar processes. Notice that the Eco-indicator 99 for resources only considers two impact categories for the damages caused by extraction of minerals and fossil fuels; however, other damages caused by the depletion of resources such as extraction of water or other resources are not considered with this methodology.

Table 10. Values for Damages Associated with Bioethanol Production

emissions to air	compound	emissions per ton of *A. jocotepecana*	associated EI-99 (points)	type of damage
1	CO_2	3.37	0.00545 per ton of emissions	0.0183 F

Table 11. Values for Damages Associated with *Ambrox* Production

emissions to air	compound	emissions per ton of *A. jocotepecana*	associated EI-99 (points)	type of damage
1	CO_2	192.551	0.00545	1.049 F
2	NO_x	1.024	2.30, 0.445	C, H
3	SO_x	0.062	1.42, 0.0812	C, H
occupation	factor × m^2 × y		0.0655	I
conversion	factor × m^2		1.96	I
energy from coal	factor × MJ used		0.000204	K

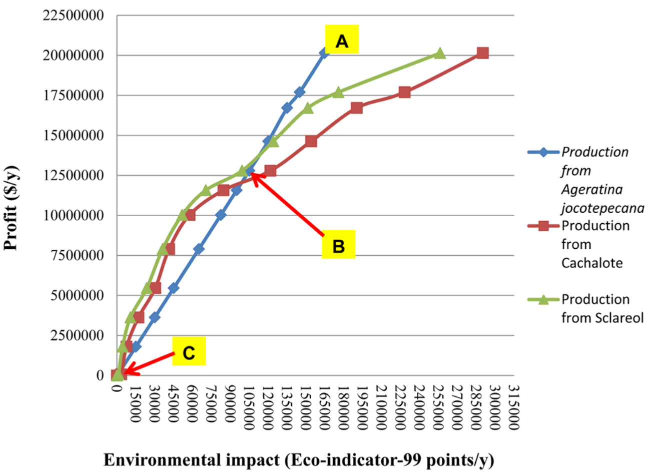

Figure 5. Trade-offs between economic and environmental objectives in the SC.

Thus, this is a multiobjective optimization problem that can be stated as follows

$$\text{Objective function} = (\max \text{profit}; \min \text{EI}) \tag{43}$$

The multiobjective optimization problem was solved using the constraint method. The model is a mixed-integer linear programming problem (MILP), which was coded in the software GAMS,[28] and solved with the solver CPLEX in a computer with an Intel Core i7 processor at 2.67 GHz with 8 GB of RAM in an average of 1 s of CPU time. The size for the model formulation includes 166 continuous variables, 155 single equations, and 24 discrete variables.

RESULTS AND DISCUSSION

The information for the different municipalities considered for the *Ageratina jocotepecana* cultivation were taken from INEGI.[29] This way, the available land in each municipality is 559,000 ha in Hidalgo, 209,000 ha in Pátzcuaro, 102,000 ha in Quiroga, 215,000 ha in Zacapu, and 241,000 ha in Zitácuaro. Furthermore, the current land cultivated with *A. jocotepecana* in each municipality is 5.59, 2.09, 1.02, 2.15, and 2.41 ha for Hidalgo, Pátzcuaro, Quiroga, Zacapu, and Zitácuaro, respectively. A preliminary analysis shows that the total land required to satisfy the total demand of *Ambrox* is 2369 ha. This area represents only 2.8% of the land used for agriculture in Quiroga, which is the main municipality with *A. jocotepecana* and is the one selected by the optimization model for *A. jocotepecana* cultivation, which includes the installation of a central processing facility in the city of Morelia. Furthermore, the required area for cultivation of *A. jocotepecana* does not exceed 1.6% of the

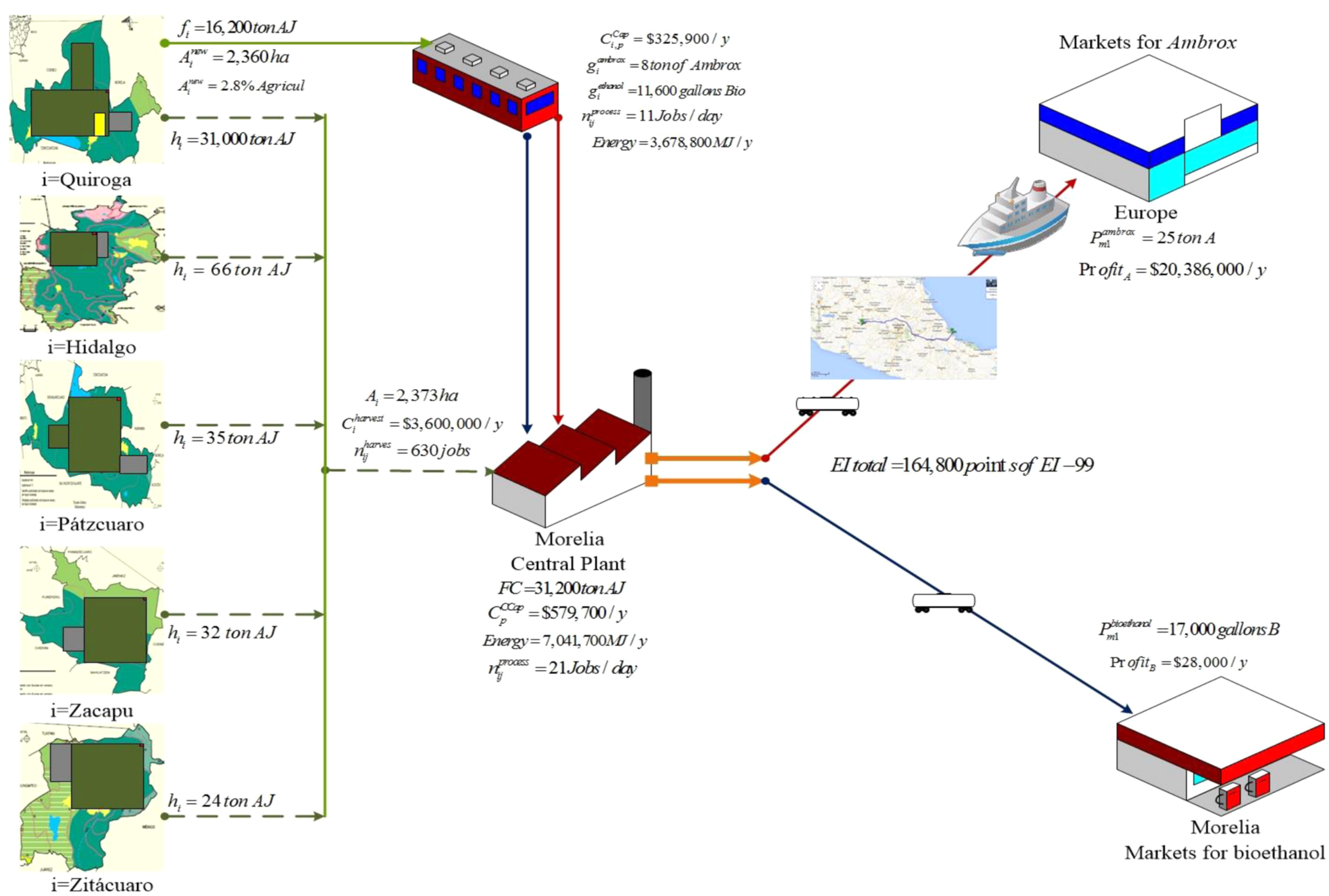

Figure 6. Configuration for the supply chain associated with the optimal economic solution (Scenario A).

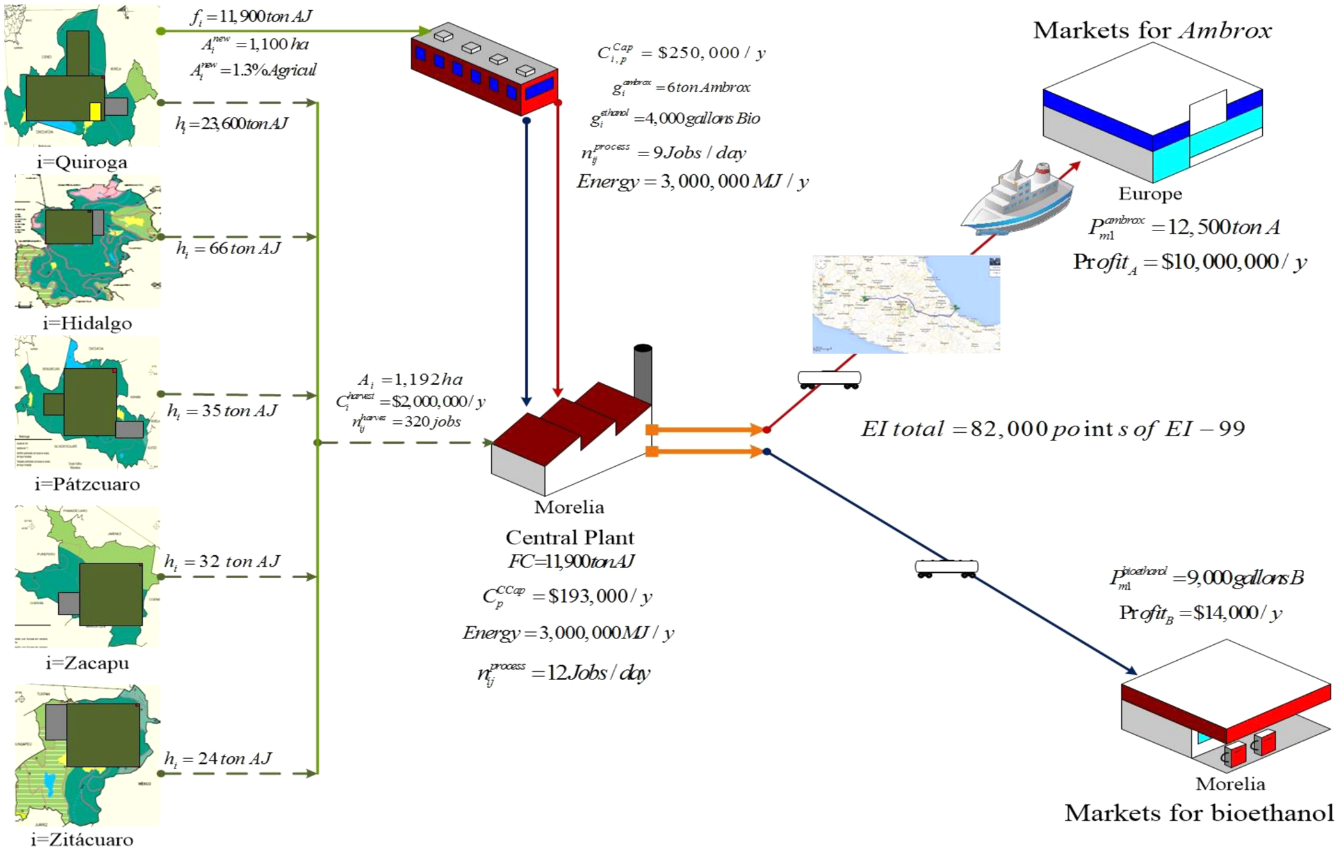

Figure 7. Configuration for the supply chain associated with Scenario B.

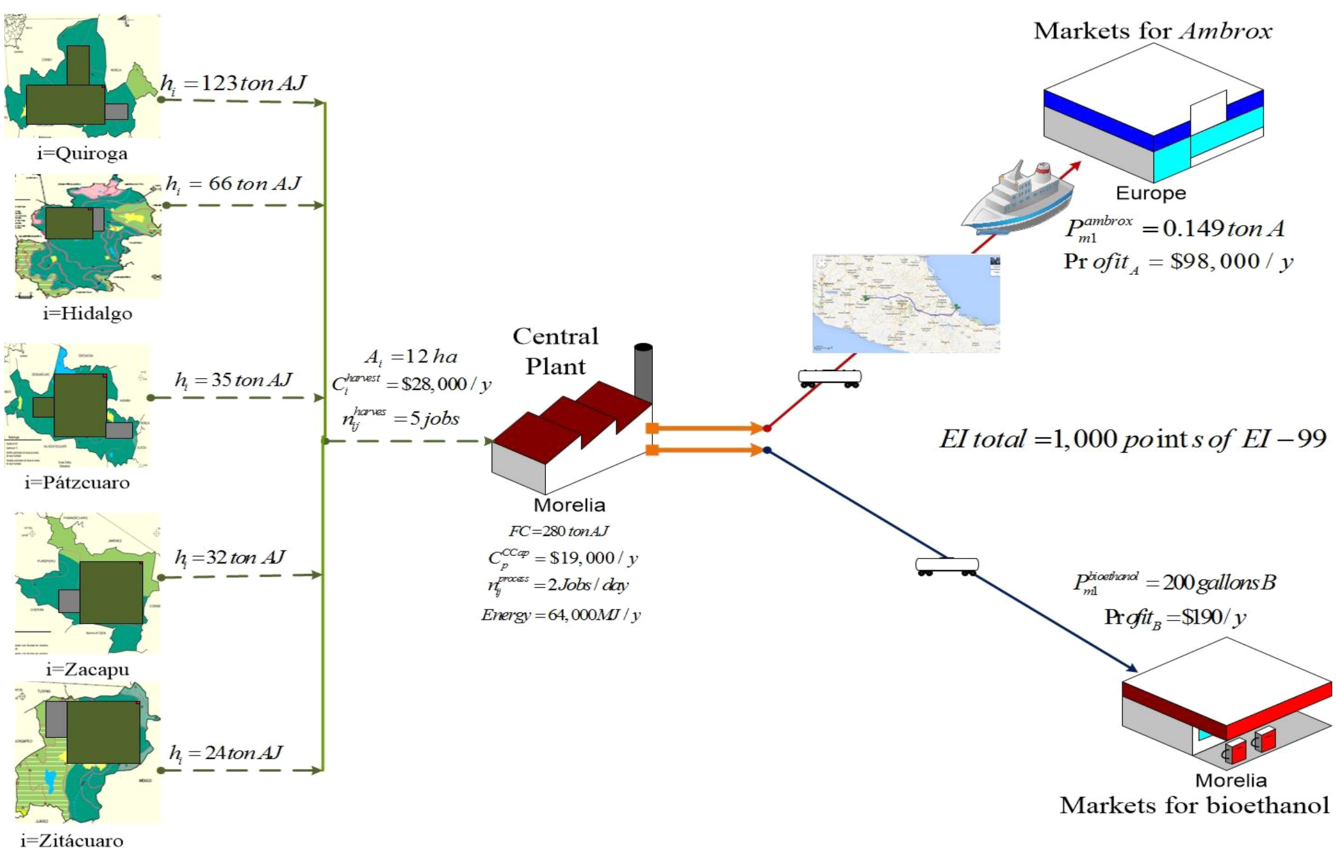

Figure 8. Configuration for the supply chain associated with Scenario C.

Table 12. Economic Results Comparison ($/y)

solution/activity	farming	transport of raw material	processing	transport products	final earnings
A	3,690,000	30,000	824,000	69,000	20,168,000
B	1,848,000	15,000	452,000	34,000	10,023,000
C	20,000	–	93,000	–	–

Table 13. Results for Generated Jobs

solution/sector	farm	industrial	total
A	633	43	676
B	317	22	339
C	4	2	6

available land in any other municipality. With this area, is possible to achieve an annual production of 25 tons of *Ambrox* and 17,823 gallons of bioethanol.

Figure 5 shows the trade-offs between the economic and environmental objectives considered in the optimization formulation. Point A corresponds to the solution with the maximum profit (but with the maximum environmental impact), whereas point C corresponds to the solution with the minimum environmental impact (with the minimum profit). Also, Figure 5 shows a comparison between the three most common ways to produce the fixative in the perfume industry: production from the Cachalot killing and synthetic chemical process from Sclareol and from *A. jocotepecana*.

For the best economic solution (point A of Figure 5), the total number of jobs generated is 633, which represents a significant contribution in this aspect. The economic objective function considers all the activities involved in the supply chain. First, the harvesting stage ($3,690,000/y) accounts for land preparation, fertilization, sowing, and cutting. Then, the transportation cost for the raw materials to the processing facilities is $30,000/y. The costs of production in the central and distributed plants are $362,000/y and $462,000/y, respectively, and finally, the transportation cost of products is $68,000/y. This way, the supply chain obtains a gross profit for the sale of *Ambrox* and bioethanol of $20,386,000/y and $28,000/y, respectively. The total environmental impact was evaluated by the Eco-indicator 99 methodology. For scenario A, the environmental impact is 164,850 points of Eco-indicator 99, which encloses all the activities from the cultivation of *A. jocotepecana* to the final product. The aforementioned value is composed by 210,580 points of Eco-indicator 99 per year for obtaining the raw material, 3358 points for the production of bioethanol, and 347 points for production of *Ambrox*, minus 45,730 points for the positive environmental impact that involves CO_2 fixed by crops. Figure 6 shows the supply chain configuration for the best economic solution identified as solution A. For this solution, only the municipality of Quiroga is selected as a cultivation site, whereas a central processing facility is required in the city of Morelia (48 km away from Quiroga) and a distribution facility is installed in Quiroga.

Solutions B (configuration shown in Figure 7) and C (configuration shown in Figure 8) in the Pareto front represent different scenarios in which the environmental impact is reduced; however, the earnings also decrease proportionally. This means that these solutions cannot satisfy the demand of 25 tons of *Ambrox*. On the other hand, solution C is the solution where no new land is used for the production of *A. jocotepecana*. An alternative to reduce the environmental impact without sacrificing the production is the use of alternative energy sources.

Tables 12, 13, and 14 show a comparison of the three solutions identified in Figure 5. In Table 14, the impact of the production and transportation of raw materials, bioethanol, and Ambrox are summed to obtain the subtotal, and then the amount of fixed CO_2 is subtracted from this value to obtain the total impact.

■ CONCLUSIONS

A multiobjective mathematical programming model for the optimal synthesis of the supply chain for the production of *Ambrox* from *Ageratina jocotepecana* has been developed. The supply chain includes cultivation of *Ageratina jocotepecana* in additional lands and the substitution of precursors for perfume fixatives. The results show the potential of the route due to the use of a simplified chemical route coupled with an appropriate SC. The implementation of the new route in the State of Michoacán, México, offers positive economic and social impacts (enhanced profits and generated jobs). On the other hand, there are environmental concerns associated with the new SC. The major impact is associated with the production of the raw materials due to the change of land. An alternative to overcome this problem is using existing land designated for agricultural activities as well as sharing crops. Additionally, the energy associated with the process can be provided by renewable sources to reduce the negative environmental impact.

■ NOMENCLATURE

This section is divided as parameters and variables, the parameters correspond to data in the optimization formulation, whereas the variables correspond to degrees of freedom that are optimized.

Parameters

$A_i^{existing}$ Existing area with wild *Ageratina jocotepecana* in site *i*, (ha)

A_i^{max} Total area in site *i*, (ha)

$C_{i,p}^{F}$ Fixed cost associated with the capacity of each preprocessing facility, ($/y)

$C_{cen,p}^{F}$ Fixed cost associated with the capacity of central facility, ($/y)

C_{cen}^{V} Variable cost associated with the central facility, ($)

C_i^{V} Variable cost associated with each preprocessing facility, ($)

$C_i^{harvest}$ Unit cost for cultivation of *Ageratina jocotepecana*, ($/ha)

$C_i^{process}$ Unit preprocessing cost, ($/ton)

Table 14. Results for Environmental Impact (Eco-indicator 99/y)

solution/sector	raw material	bioethanol	*Ambrox*	sub-total	fixed CO_2	total
A	210,580	3358	347	214,285	49,439	164,846
B	105,290	1679	174	107,143	24,719	82,424
C	790	12	4	806	66	740

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$C_i^{\text{trans}-Ambrox}$ Unit processing cost for *Ambrox* in the central processing facility, ($/ton)
$C_i^{\text{transpo}-Ambrox}$ Unit transportation cost for *Ambrox* from distributed to central processing facilities, ($/ton)
$C_{\text{im2}}^{\text{transpo}-\text{ethanol}}$ Unit bioethanol transportation cost, ($/gallon)
$C_i^{\text{transpo}-\text{plant}}$ Unit transportation cost for raw materials, ($/ton)
$C_{\text{m2}}^{\text{transpo}-\text{ethanol}}$ Unit transportation cost for bioethanol from processing facilities to markets, ($/gallon)
$C_{\text{m1}}^{\text{transpo}-Ambrox}$ Unit transportation cost for *Ambrox* from processing facilities to markets, ($/ton)
$F_{Aj,\text{central,p}}^{\text{lower}}$ Minimum processed stem of *Ageratina jocotepecana* at central facility, (ton)
$F_{Aj,i,\text{p}}^{\text{lower}}$ Minimum processed stem of *Ageratina jocotepecana* in each preprocessing facility, (ton)
$F_{Aj,\text{central,p}}^{\text{upper}}$ Maximum processed *Ageratina jocotepecana* in the central facility, (ton)
$F_{Aj,i,\text{p}}^{\text{upper}}$ Maximum processed stem flux of *Ageratina jocotepecana* in each preprocessing facility, (ton)
n_i^{harvest} Unit generated jobs for cultivation of *Ageratina jocotepecana*, (jobs/ha)
n_i^{process} Unit processing and transportation jobs for the central processing facility, (jobs/ton)
$n_i^{transpo-Ambrox}$ Unit generated jobs for transportation of *Ambrox* from the distributed to the central processing facility, (Jobs/ton)
$n_{\text{i,m2}}^{\text{transpo}-\text{ethanol}}$ Unit generated jobs for transportation from the distributed to the central processing facility, (jobs/ton)
$n_i^{\text{transpo}-\text{plant}}$ Unit generated jobs for transportation for *Ageratina jocotepecana* to the central processing facility, (jobs/ton)
$n_{\text{m1}}^{\text{transpo}-Ambrox}$ Unit generated jobs for the transportation of *Ambrox* to the markets, (jobs/ton)
$n_{\text{m2}}^{\text{transpo}-\text{ethanol}}$ Unit generated jobs for transportation of bioethanol to markets, (jobs/ton)
$\text{Price}_{\text{m1}}^{Ambrox}$ Sale price for *Ambrox* in the market, ($/ton)
$\text{Price}_{\text{m2}}^{\text{ethanol}}$ Sale price for bioethanol in market, ($/gallon)
P^{Ambrox} *Ambrox* production in the central plant, (ton)
P_{ethanol} Bioethanol production in the central plant, (gallon)
P_{m1}^{Ambrox} Demand of *Ambrox*, (ton)
$P_{\text{m2}}^{\text{ethanol}}$ Demand of bioethanol, (gallon)
α_i Percent of stems produced by ha in site *i*, (ton/ha)
β_i^{Ambrox} Conversion factor from stems to *Ambrox*, (dimensionless)
β_i^{ethanol} Conversion factor from stems to bioethanol, (dimensionless)
γ^{Ambrox} Conversion factor from stems to *Ambrox* in central plant, (dimensionless)
γ^{ethanol} Conversion factor from stems to bioethanol in central plant, (dimensionless)

Variables

A_i Cultivation area, (ha)
A_i^{new} New area required, (ha)
$C_{\text{prepropla},i}^{\text{capprocess}}$ Capital cost associated with each preprocessing facility, ($)
$C_{\text{central}}^{\text{capprocess}}$ Capital cost associated with central facility, ($)
Cost Total capital cost, ($)
$\text{DF}_{Aj,i,\text{p}}$ Disaggregated variable for flux stem processed in the preprocessing facility, (ton/y)
$\text{DC}_{i,p}^{Cap}$ Disaggregated variable for capital cost associated with preprocessing facility, ($)
$\text{EI}_{\text{Global}}$ Environmental impact generated by the supply chain, (Ecopoints-99)
EI_{Ambrox} Environmental impact generated by the *Ambrox* production, (Ecopoints-99/ton)
$\text{EI}_{\text{bioethanol}}$ Environmental impact generated by the bioethanol production, (Ecopoints-99/gallon)
$\text{EI}_{\text{rawmaterial}}$ Environmental impact generated by the raw material cultivation, (Ecopoints-99/ton)
F_i Produced *Ageratina jocotepecana* in site *i*, (ton/ha)
f_i Flow rate for the stems sent to the distributed processing facilities, (ton)
$F_{Aj,i}$ Flux stem processed in each preprocessing facility, (ton)
F_{central} Stem processed in the central facility, (ton)
g_i^{Ambrox} *Ambrox* produced in preprocessing facilities, (ton)
g_i^{ethanol} Bioethanol produced in preprocessing facilities, (gallon)
h_i Flow rate for the stems sent to the central processing facility, (ton)
M^{Ambrox} Total *Ambrox* produced, (ton)
M^{ethanol} Total bioethanol produced, (gallon)
N_{jobs} Total generated jobs, (jobs)
NP Gross profit, ($)
$P_{\text{m1}}^{\text{max ambrox}}$ Demand of *Ambrox* that is satisfied by the sales, (ton/y)
$P_{\text{m2}}^{\text{max ethanol}}$ Demand of bioethanol that is satisfied by the sales, (gallon/y)
Profit Total profit, ($/y)
S_{m1}^{Ambrox} Amount of *Ambrox* that is sold, (ton/y)
$S_{\text{m2}}^{\text{ethanol}}$ Amount of bioethanol that is sold, (gallon/y)
Sales Sales, ($/y)
Y_{p}^{c} Binary variable for the existence or not of central facility, (dimensionless)
$Y_{\text{p},i}$ Binary variable for the existence or not of preprocessing facility, (dimensionless)

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Notes

The authors declare no competing financial interest.

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