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# Marginalization index as social measure for Acetone-Butanol-Ethanol supply chain planning

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ABSTRACT

Most of methodologies for evaluating supply chain have been focused on environmental and economic criteria. Even though, social impact has been addressed in some methodologies, these methodologies have not considered the location where social impact takes place, which is a crucial issue when the social impact is measured. Therefore, the research purpose is to consider the social impact as a function of the supply chain facilities location. This is accomplished through a multi-objective approach for planning of a biomass supply chain considering simultaneously several objective functions: a) the social impact in function the location where it occurs, b) net profit and c) net $CO_2$ emissions. Specifically, proposed mathematical model considers a social objective function based on the marginalization index. Multi-objective approach was addressed via generating several Pareto curves to illustrate the tradeoff between the considered objectives. Maximum reached profit was around $US 13,572 Million per year that can be obtained with two different pairwise analysis. Nevertheless, if the social benefit is maximized, the profit decrease until $US 6000 Million per year. Therefore, results indicate that supply chain entity's location has a crucial effect in the social impact. Additionally, a direct correlation between social functions other objectives was not observed. This approach addressed the lack of studies for the supply chain planning involving social impact functions, which should be multi-factorial. The proposed approach is applied to an important industrial process, the Acetone-Butanol-Ethanol (ABE) process, to contribute to the bioenergy sector developing.

## Author contributions

**Santibañez-Aguilar, J.E.:** Contextualization, Methodology, Software, Writing – original draft, Investigation. **Quiroz-Ramírez, J.J.:** Validation, Investigation, Writing – review & editing. **Sánchez-Ramírez, E.:** Conceptualization, Validation, Investigation, Writing – review & editing. **Segovia-Hernández, J.G.:** Conceptualization, Validation, Investigation, Writing – review & editing. **Flores-Tlacuahuac, A.F.:** Resources, Writing – review & editing. **Ponce-Ortega, J.M.:** Conceptualization, Writing – review & editing.

## 1. Introduction

Climate change and global warming have become serious social, economic and environmental problems caused by different human activities linked with drastic augments in energy consumption as well as population. In this regard, the global trend to address these problems has been the use of low carbon emission technologies as well as decarbonization ([1,2]); such as solar and wind energy as well as partial substitution of conventional fossil fuels. In fact, prior of the COVID-19 crisis [3], projected that energy demand would increase by 12% between 2019 and 2030, which 80% of the electricity demand growth would correspond to renewable energy if all announced policy intentions and targets are maintained. In this way, even though the energy demand issue and environmental problem due to GHGE have been addressed by installing renewable energy production supply chains or promoting more renewable energy using, the social impact has not been widely discussed.

Substitution of fossil fuels by biofuels is promising since it would

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**List of abbreviations**

| | |
|---|---|
| ABE | Acetone-Butanol-Ethanol |
| AMPL | A Mathematical Programming Language |
| BARON | Branch-and-Reduce Optimization Navigator |
| CONAPO | National Council of Population |
| DICOPT | Discrete and Continuous Optimizer |
| EMISS | Objective function for $CO_2$ eq emissions |
| GAMS | General Algebraic Modelling System |
| GIS | Geographic Information Systems |
| INEGI | National Institute for Statistic, Geographic and Informatic for Mexico |
| IPOPT | Interior Point Optimizer |
| MI | Marginalization Index |
| MILP | Mixed Integer Linear Programming |
| MINLP | Mixed Integer Non-Linear Programming |
| NP | Objective function for net profit |
| PEMEX | Mexican Petroleum Company |
| SADER | Mexican Ministry of Agricultural and Rural Development |
| SCT | Mexican Ministry of Transportation and Communications |
| SENER | Mexican Ministry of Energy |
| SOL | Social objective function associated to locations |

*NomenclatureParameters*

| | |
|---|---|
| $A_{r,q}$ | Fixed term for the capital investment function in processing plant $r$ and the processing interval $q$ before to be annualized ($\$USD$) |
| $B_{r,q}$ | Variable term for the capital investment function in processing plant $r$ and the processing interval $q$ before to be annualized ($\$USD \cdot year \cdot Mg^{-1}$) |
| $C_m^{transp-M}$ | Unitary transportation cost for raw materials ($\$USD \cdot Mg^{-1} \cdot km^{-1}$) |
| $C_p^{transp-P}$ | Unitary transportation cost for products ($\$USD \cdot Mg^{-1} \cdot km^{-1}$) |
| $C_r^{operating}$ | Unitary operating cost in processing plants ($\$USD \cdot Mg^{-1}$) |
| $C_{c,p}^{product}$ | Unitary product price in the consumption region $c$ ($\$USD \cdot Mg^{-1}$) |
| $C_{m,s}^{biomass}$ | Unitary cost for biomass in suppliers ($\$USD \cdot Mg^{-1}$) |
| $d_{s,r}^{S-R}$ | Distance between biomass suppliers and processing plants ($km$) |
| $d_{r,c}^{R-C}$ | Distance between processing plants and consumption centers ($km$) |
| $E_m^{transp-M}$ | Unitary emissions for raw material transportation ($EmissionsCO_2eq \cdot Mg^{-1} \cdot km^{-1}$) |
| $E_p^{transp-P}$ | Unitary emissions for product transportation ($EmissionsCO_2eq \cdot Mg^{-1} \cdot km^{-1}$) |
| $E_r^{operating}$ | Unitary emissions for biomass processing ($EmissionsCO_2eq \cdot Mg^{-1}$) |
| $E_p^{product}$ | Unitary emissions according product use ($EmissionsCO_2eq \cdot Mg^{-1}$) |
| $E_m^{biomass}$ | Unitary emissions associated to the biomass production ($EmissionsCO_2eq \cdot Mg^{-1}$) |
| $F_{m,s}^{\max}$ | Maximum raw material $m$ to be used from the biomass supplier $s$ ($Mg \cdot year^{-1}$) |
| $F_{m,s}^{\min}$ | Minimum raw material $m$ to be used from the biomass supplier $s$ ($Mg \cdot year^{-1}$) |
| $F_r^{Margin-plants}$ | Marginalization index for processing plants |
| $F_{c,p}^{Demand}$ | Product demand of product $p$ in consumption region $c$ ($Mg \cdot year^{-1}$) |
| $F_{r,q}^{MAX-cap}$ | Upper limit for the processing capacity interval $q$ in the processing plant $r$ ($Mg \cdot year^{-1}$) |
| $F_{r,q}^{MIN-cap}$ | Lower limit for the processing capacity interval $q$ in the processing plant $r$ ($Mg \cdot year^{-1}$) |
| $F_s^{Margin-harvesting}$ | Marginalization index for harvesting sites |
| $KF$ | Annualization factor for the capital investment function ($year^{-1}$) |
| $TotalSites$ | Total harvesting sites |
| $TotalPlants$ | Total processing plants |
| $x_{m,r}^{R}$ | Cellulose composition for the received raw material $m$ to the processing plant $r$ |
| $\alpha_{r,p}^{cell-P}$ | Cellulose to product ratio ($Mg\ product \cdot Mg\ cellulose^{-1}$) |

*Variables*

| | |
|---|---|
| $BC$ | Total biomass cost to be used in the production system ($\$USD \cdot year^{-1}$) |
| $BE$ | Total emissions for biomass production ($EmissionsCO_2eq \cdot year^{-1}$) |
| $CC$ | Annual capital investment to be considered in the net profit function ($\$USD \cdot year^{-1}$) |
| $EMISS^{MAX}$, $EMISS^{MIN}$, $EMISS^{solution}$ | Maximum, minimum and solution values for EMISS objective |
| $EP$ | Total emissions for product use ($EmissionsCO_2eq \cdot year^{-1}$) |
| $F_{m,s}^{used}$ | Used raw material $m$ from the harvesting sites $s$ ($Mg \cdot year^{-1}$) |
| $F_{m,s,r}^{S-R}$ | Distributed raw material $m$ from biomass suppliers to processing facilities ($Mg \cdot year^{-1}$) |
| $F_{m,r}^{R}$ | Total received raw material $m$ into the processing plant $r$ ($Mg \cdot year^{-1}$) |
| $F_r^{feed}$ | Total cellulose in the processing plant $r$ considering all received raw material ($Mg \cdot year^{-1}$) |
| $F_{r,p}^{P}$ | Produced product $p$ in the processing plant $r$ ($Mg \cdot year^{-1}$) |
| $F_{r,p,c}^{R-C}$ | Distributed product from processing plant to consumption center ($Mg \cdot year^{-1}$) |
| $F_{c,p}^{C}$ | Received product $p$ in consumption region $c$ ($Mg \cdot year^{-1}$) |
| $F_{r,q}^{capq}$ | Annual process capacity according the processing interval $q$ and facility $r$ ($Mg \cdot year^{-1}$) |
| $F_r^{cap}$ | Annual process capacity considering all capacity production intervals $q$ ($Mg \cdot year^{-1}$) |
| $OC$ | Annual operating cost for processing in plants ($\$USD \cdot year^{-1}$) |
| $OE$ | Annual emissions for processing in plants ($EmissionsCO_2eq \cdot year^{-1}$) |
| $Term^{harvesting}$ | Term for harvesting sites for social objective |
| $Term^{plants}$ | Term for processing plants for social objective |
| $NetEmission$ | Total net emissions for the considered supply chain ($EmissionsCO_2eq \cdot year^{-1}$) |
| $NP^{MAX}$, $NP^{MIN}$, $NP^{solution}$ | Maximum, minimum and solution values for NP objective |
| $SatisfactionEMISS^{solution}$ | Percentage of satisfaction for EMISS objective |
| $SatisfactionNP^{solution}$ | Percentage of satisfaction for NP objective |
| $SatisfactionSOL^{solution}$ | Percentage of satisfaction for SOL objective |
| $TC$ | Total transportation cost into supply chain ($\$USD \cdot year^{-1}$) |
| $TE$ | Total emissions concerning transportation ($EmissionsCO_2eq \cdot year^{-1}$) |
| $x_r^{cel}$ | Cellulose composition in the processing plant $r$ considering all received raw material |

*Binary variables*

| | |
|---|---|
| $y_{m,s}^{used}$ | Binary variable to define if the raw material $m$ from biomass supplier $s$ is used |
| $y_{r,q}^{cap}$ | Binary variable to define if a processing interval is considered for the capital investment function |

allow a gradual transition to decarbonized production system. In this respect, supply chain planning is straightly associated to supply chain assessment, which can be via economic, environmental and social objectives. Nevertheless, social objectives are extremely difficult to evaluate because social aspects are multifactorial, and they depend on the supply chain facilities location. For instance, biofuels supply chains have been studied in order to maximize the net profit ([4]), minimize the global emissions ([5]), maximize the new jobs. ([6]), between other objectives; however, these papers have not considered the social impact as their main objective.

It is worth noting that inclusion of social and economic issues into the supply chain planning problem is according with the United Nations Sustainability Development Goals such as: "End poverty in all its forms everywhere" ([7]) because planning solution can be focused on developing poor and marginalized regions. Furthermore, considering of alternative energy sources such as biofuels production is according with another United Nations Sustainability Development Goals such as: "Ensure access to affordable, reliable, sustainable and modern energy for all" ([7]).

Therefore, this paper addresses these two United Nations goals because presented approach is applied to a case study with high global interest such as the (Acetone-Butanol-Ethanol) ABE process, since bioethanol and biobutanol are two promising biofuels in the world for the transportation field. In addition, this work presents a multi-objective mathematical model for the supply chain planning considering as the main objective a social function associated to the location to carry out the supply chain assessment in a whole manner.

Novelty of this paper is that mathematical formulation considers economic, environmental and social objectives simultaneously, in which the social objective function is a multifactorial function that is directly associated to supply chain facility locations (based on the marginalization index). It is important to mention that other works do not include the location into the social objective directly. Thus, in this paper the supply chain facility locations play a crucial role in the planning problem since supply chain planning is focused to select sites with high marginalization level to promote the development of poor and marginalized communities, also assessing economic and environmental issues.

## 2. Literature review

Along this section, several works concerning supply chain planning, sustainability assessing, importance of renewable energy and biofuels production are discussed. It should be noted that discussion objective is to highlight the novelty of the presented paper and to provide context about matters and drawbacks when a supply chain problem is addressed.

### *2.1. Biofuels as alternative for transport decarbonization*

As mentioned, decarbonization of technologies is a clear global trend to address the climate change and global warming problems. Some of the main efforts, have been focused on the transportation sector because vehicles can substantially contribute to emissions of carbon dioxide and other pollutants such as hydrocarbons, carbon monoxide, nitrogen oxides, etc [8]. For example [9], have reported emission factors for carbon monoxide and nitrogen oxides under real operating conditions for diesel passenger buses in Mexico. Also [10], estimated that off-road and on-road vehicles could have contributed about 38% of the total black carbon emissions in Mexico in 2013.

An interesting alternative to address this problem is the gradual substitution of fossil fuels by biofuels such as biodiesel, ethanol and butanol [11]. Regarding ethanol, several authors have mentioned that ethanol is a promising gasoline substitute based on different reasons. For instance, according to Ref. [12], ethanol as fuel has been proved as a renewable and clean energy source. In addition [13], mentioned that ethanol has an octane number higher than gasoline; therefore, ethanol-gasoline blends have an octane number higher than conventional gasoline. Also [14], stated that the oxygen content in ethanol increases the combustion efficiency in gasoline-ethanol blends.

Currently, the most mature technology for the production of butanol from fermentation uses strains from the Clostridium family. The advantage of using any of these bacteria is that they can use sugars of five or six carbons interchangeably, commonly both produced in the hydrolysis process. Conversely, the yeasts traditionally charged with producing ethanol can only use six-carbon sugars [15]. The yields associated with the production of ethanol are slightly higher than those presented in the production of butanol. However, there are a few factors why butanol could be considered a superior fuel to ethanol. For example, the energy content of butanol is higher than that present in ethanol, obviously closer to the content in gasoline. Additionally, some physicochemical properties put butanol one step above ethanol; it is less volatile, less flammable, less dangerous to handle, and less water-related. Due to the low vapor pressure, butanol can be transported through the existing pipeline infrastructure. Additionally, butanol can be blended in any proportion with gasoline, it could even be used directly in any car without the need for any mechanical modification or packaging [15]. On the contrary, to use a gasoline-ethanol blend without suffering engine damage in the medium and long term, FlexFuel type engines are needed. FlexFuel engines can be used with a mixture of up to 85% ethanol (E85). However, the typical ethanol-gasoline blend has an energy power 15–27% lower than gasoline [16]. Also, butanol could be used as biofuel because its octane number is comparable with gasoline octane number and the lower heating value of n-butanol is higher than the one of ethanol [17].

Therefore, butanol and ethanol have shown potential to substitute gasoline or to be used in gasoline blends. This way, both compounds can be produced via the ABE (Acetone-Butanol-Ethanol) process, which is based on fermentation of lignocellulosic materials. The ABE process might have an advantage over others because most of chemical processes need to separate their final products and the separation process could be too expensive; nevertheless, according to Ref. [17] the separation in the ABE process could be unnecessary because butanol and ethanol could be used as fuels.

Even though ethanol and butanol have interesting properties as fuels, both are mainly produced via fermentation and these processes achieve low butanol or ethanol concentrations, which could not be economically attractive. Although [15,18], showed that butanol production could be economically attractive if fermentation technologies use agricultural residues.

According to specialized reports, there are two problems associated with ABE fermentation: 1. The use of diluted sugars that generate diluted products, and 2. The high energy requirement to carry out the separation of the product of interest. In this sense, efforts have been oriented in the area of process intensification, trying to increase the feasibility of the ABE process. For example [19], proposed an integrated saccharification-fermentation reactor that has improved efficiency in the fermentation section. Furthermore [20,21], proposed a considerable number of intensified alternatives for separation, with the objectives of reducing energy requirements. Note in both cases that the use of intensified technology allows to overcome the current conventional technology.

Lastly, in spite of butanol and ethanol being promising fuels, it is needed to assess the entire supply chain under several sustainability criteria.

### *2.2. Marginalization index as a multifactorial index*

Particularly for Canada [22], stated that marginalization index is a multifaceted index, which allows examining multiple dimensions of marginalization and their effects on health and other social outcomes. Also, Mexican government has considered several factors for the marginalization index such as: a) percentage of population over 15 years

**Table 1**
Marginalization index value and its components for all federal states in Mexico for 2015. CONAPO, (2020) [24].

| Federal state | A[a] | B[a] | C[a] | D[a] | E[a] | F[a] | G[a] | H[a] | I[a] | MI[a] |
|---|---|---|---|---|---|---|---|---|---|---|
| Aguascalientes | 2.6 | 11.89 | 0.67 | 0.3 | 0.81 | 21.86 | 0.75 | 25.16 | 34.6 | −0.89 |
| Baja California | 1.96 | 10.46 | 0.26 | 0.47 | 2.82 | 23.03 | 1.15 | 10.35 | 22.85 | −1.1 |
| Baja California Sur | 2.51 | 11.59 | 0.38 | 1.14 | 7.15 | 26.23 | 4.08 | 15.62 | 22.37 | −0.6 |
| Campeche | 6.68 | 18.56 | 4.08 | 1.59 | 6.49 | 37.93 | 2.95 | 30.88 | 40.69 | 0.46 |
| Coahuila | 1.99 | 9.56 | 0.62 | 0.29 | 1.67 | 23.62 | 0.66 | 12.15 | 27.94 | −1.1 |
| Colima | 3.9 | 15.24 | 0.38 | 0.38 | 0.96 | 25.65 | 2.45 | 14.47 | 31.18 | −0.73 |
| Chiapas | 14.98 | 31.71 | 2.9 | 2.49 | 13.45 | 44.46 | 11.78 | 57.86 | 62.46 | 2.41 |
| Chihuahua | 2.67 | 12.65 | 1.4 | 1.81 | 2.39 | 22.16 | 1.76 | 17.05 | 34.77 | −0.6 |
| Distrito Federal | 1.49 | 6.62 | 0.04 | 0.04 | 1.1 | 19.19 | 0.47 | 0.67 | 28.26 | −1.45 |
| Durango | 3.17 | 14.5 | 3.68 | 2.63 | 3.26 | 24.58 | 4.33 | 36.19 | 39.16 | 0.05 |
| Guanajuato | 6.39 | 19.12 | 3.31 | 0.68 | 4.13 | 25.36 | 2 | 34.67 | 37.41 | −0.07 |
| Guerrero | 13.73 | 27.25 | 13.03 | 2.4 | 15.64 | 42.11 | 14.86 | 49.68 | 53.29 | 2.56 |
| Hidalgo | 8.26 | 18.13 | 3.09 | 1.12 | 5.83 | 28.17 | 3.19 | 58.71 | 46.22 | 0.5 |
| Jalisco | 3.55 | 14.9 | 0.86 | 0.34 | 1.84 | 22.12 | 1.59 | 17.5 | 29.4 | −0.82 |
| México | 3.37 | 11.77 | 1.68 | 0.38 | 4.03 | 28.53 | 1.92 | 19.11 | 35.28 | −0.57 |
| Michoacán | 8.35 | 25.35 | 2.32 | 0.81 | 4.26 | 28.05 | 5.9 | 40.58 | 44.88 | 0.5 |
| Morelos | 4.99 | 15.09 | 1.03 | 0.44 | 5.81 | 27.04 | 3.88 | 24.65 | 42.08 | −0.2 |
| Nayarit | 5.07 | 17.56 | 4.66 | 2.54 | 4.36 | 27.63 | 3.92 | 39.14 | 37.96 | 0.31 |
| Nuevo León | 1.64 | 8.38 | 0.16 | 0.12 | 1.36 | 23.09 | 0.8 | 6.7 | 16.15 | −1.39 |
| Oaxaca | 13.65 | 29.22 | 2.44 | 2.87 | 13.05 | 38.33 | 13.44 | 61.51 | 49.46 | 2.12 |
| Puebla | 8.39 | 21.32 | 1.58 | 0.88 | 6.94 | 35.27 | 5.69 | 38.5 | 52.16 | 0.69 |
| Querétaro | 4.57 | 13.01 | 2.93 | 0.67 | 3.23 | 24.21 | 1.52 | 39.07 | 25.92 | −0.49 |
| Quintana Roo | 3.9 | 13.32 | 2.19 | 1.11 | 2.7 | 36.31 | 2.41 | 14.36 | 28.32 | −0.37 |
| San Luis Potosí | 6.33 | 18.87 | 2.34 | 2.29 | 10.68 | 25.21 | 5.56 | 40.08 | 43.64 | 0.58 |
| Sinaloa | 4.18 | 16.82 | 2.57 | 0.52 | 2.99 | 30.37 | 2.85 | 32.85 | 32.7 | −0.24 |
| Sonora | 2.19 | 11.15 | 1.05 | 1.05 | 2.52 | 26.63 | 2.61 | 17.39 | 29.93 | −0.7 |
| Tabasco | 5.4 | 17.25 | 1.81 | 0.43 | 10.1 | 32.5 | 3.69 | 53.65 | 36.96 | 0.3 |
| Tamaulipas | 3.03 | 13.35 | 0.37 | 0.73 | 2.51 | 28.69 | 1.52 | 13.92 | 37.39 | −0.62 |
| Tlaxcala | 3.98 | 12.6 | 1.36 | 0.47 | 1.14 | 32 | 2 | 36.4 | 51.47 | −0.2 |
| Veracruz | 9.51 | 25.04 | 1.53 | 1.62 | 13.39 | 32.03 | 6.84 | 46.2 | 49.68 | 1.14 |
| Yucatán | 7.47 | 21.17 | 10.1 | 1.08 | 1.64 | 36.42 | 1.67 | 26.27 | 47.6 | 0.51 |
| Zacatecas | 4.42 | 19.31 | 4.17 | 0.62 | 3.13 | 24.99 | 1.25 | 48.19 | 45.4 | 0.01 |

[a] A.- % Population older than 15 unlettered. B.- % Population older than 15 with incomplete elementary school. C.- % Inhabitants without basic services. D.- % inhabitants without electricity. E.- % inhabitants without water piping system. F.- % Houses in faraway communities. G.- % Inhabitants without pavement. H.- % Population in rural communities. I.- % Population with low per capita salary. MI.- Marginalization Index.

old with non-completed elementary education, b) percentage of population without piped water, electricity energy, sewer services, c) percentage of population over 15 years old who is illiterate and, d) percentage of population living in zones of at least 5000 inhabitants among other factors (see Ref. [23]).

In this respect, marginalization index is a multifactorial index which depends on the location where it is calculated. Moreover, marginalization index is a measure of the marginalization level for communities and locations in a geographic region. For example, for Mexico, the Mexican government provides a value for marginalization index for each federal state, municipality and community. The value for Mexican marginalization index is a comparison between marginalization level of all considered locations; in which the location with the highest marginalization index corresponds to the location with highest marginalization level.

As can be seen, marginalization index is a multifactorial parameter with adequate characteristics that can be associated to a specific location and therefore, it can be used to formulate a mathematical function, which could be applied to measure the social impact in a supply chain. In this way, an adequate mathematical function can be able to promote the selection of marginalized locations when a supply chain planning problem is addressed. For example, installation of supply chain facilities in marginalized locations can enhance the life quality of communities because of diverse reasons such as jobs generation, per capita salary augment, highway and railways construction as well as electrical grids installation. Table 1 provides the marginalization index value for different federal states in Mexico.

### *2.3. Supply chain planning problem*

The addressed problem in the paper is the biomass supply chain planning that mainly consists of determining:

- Sites where raw materials will be obtained and processed
- Locations where products will be consumed or stored
- Type of raw material to be used and product to yield
- Mass amounts of products and raw materials associated to the supply chain
- Raw material cost, transportation cost, storage cost, operational cost, capital investment as well as other associated costs or economic indicators
- Processing facility capacities
- Satisfied product demand level

In literature, several models addressing the biomass supply chain planning problem can be found. Regarding biogas and power generation supply chains [25], presented a multi-objective optimization approach for biogas supply chains considering the profit and environmental impact as objectives. Also [4], developed a novel methodology to solve the sustainable biomass supply chain planning problem [26]. addressed the optimal design and planning problem of a biomass supply chain for power generation considering various technologies [27]. presented an optimization model for planning a biomass to bioenergy sustainable supply chain including issues such as emissions of feedstocks transport, processing and distributing the bioproducts to markets. Furthermore, mathematical optimization for supply chain considering co-existence of new and existing biomass power plants was used by Ref. [28]. In addition [29], proved different optimization formulations for multi-product supply chain networks to produce biogas from manure. Moreover, an alternative to produce power from biomass in the pellets production, which was addressing by Ref. [30] considering activities from biomass residues collection until pellets combustion in power plants.

**Table 2**
Supply chain planning summary for model type, used software, solution strategy, country of case study and considered objectives.

| Supply chain type | Authors | Ref | Model type | Software | Solver | Country | Objectives |
|---|---|---|---|---|---|---|---|
| Bioenergy and biofuel supply chain | Akhtari and Sowlati, (2020) | [31] | MILP | AIMMS 4.32TM | CPLEX | Canada | Net present value |
| Biogas supply chain | Diaz-Trujillo and Nápoles-Rivera, (2019) | [25] | MILP | GAMS | BARON | Mexico | Profit and emissions |
| Biogas supply chain | Durmaz and Bilgen, (2020) | [4] | MILP | – | CPLEX | Turkey | Profit and distance |
| Fodder Supply chain | Guo et al. (2020) | [37] | MILP | – | – | Spain | Profit |
| Biomass Supply chain | Espinoza-Vázquez et al. (2020) | [38] | MILP | GAMS | BARON | Mexico | Profit and product demand |
| Biomass to power supply chain | Fattahi et al. (2020) | [26] | MILP | GAMS | CPLEX | Iran | Profit |
| Bioethanol supply chain | Gilani et al. (2020) | [32] | MILP | GAMS | CPLEX | Iran | Expected Profit, environmental effect and social performance |
| Biomass-biofuel supply chain | Soleimanian et al. (2020) | [33] | – | GAMS | – | – | Total cost and time of recovery of disrupted loading and unloading hubs and biorefineries |
| Food supply chain | Martinez-Guido et al. (2019a) | [39] | MILP | GAMS | CPLEX | Mexico | Total annual cost |
| Biomass to pellets to power supply chain | Martinez-Guido et al. (2019b) | [30] | MILP | GAMS | CPLEX | Mexico | Cost and environmental impact |
| Biofuel and biogas supply chain | Sarkar et al. (2021) | [27] | MINLP | LINGO | Lingo | – | Cost and gas emissions |
| Biomass supply chain[a] | Malladi and Sowlati, (2020) | [40] | – | – | – | Canada | Feedstocks cost and total emissions |
| Bioethanol and biodiesel supply chain | Tesfamichael et al. (2021) | [34] | MILP | IBM log | CPLEX | Ethiopia | Profit and investment cost |
| Algal biomass to biodiesel supply chain | Yadala et al. (2020) | [36] | MINLP | GAMS | CONOPT3, BARON, DICOPT, ANTIGONE, CPLEX | USA | Overall cost |
| Biomass to power supply chain | Yahya et al. (2021) | [28] | MILP | LINGO | – | Malaysia | Total cost |
| Cellulosic biofuel supply chain | Ge et al. (2021) | [35] | MILP | MATLAB | Relaxation-Induced Neighborhood Search Method | USA | Overall cost |
| Manure to biogas system | Sampat et al. (2017) | [29] | MILP | JUMP | GUROBI | USA | Demand cost, supply cost, transformation cost, transportation cost |
| Biomass to ABE supply chain | This work | | MINLP | GAMS | BARON, DICOPT | Mexico | Net profit, GHGE and social objective functions |

[a] New algorithm for bi-objective optimization.

Concerning to biofuel supply chains such as bioethanol and biodiesel and other liquid biofuels [31], proposed and hybrid model for the strategic and tactical planning of a biomass supply chain considering medium-term variations in biomass supply and demand [32]. proposed a multi-phase robust supply chain network design optimization model to produce bioethanol from sugarcane. Furthermore [33], developed a bi-objective optimization model to design a biomass to biofuel supply chain, in which the objectives were the total cost and the recovery time of disrupted facilities. A multi-period model for the supply chain planning and design minimizing the investment cost and maximizing the profit for Ethiopia was developed by Ref. [34]. Also [35], proposed a multi-period formulation incorporating 12 conversion pathways and different demand levels, minimizing the supply chain cost. Particularly for biodiesel production [36], carried out a study for the design of a supply chain network to obtain biodiesel from algae biomass considering the minimization of overall supply chain cost over a planning horizon of ten years.

Other recent supply chain models are the presented by Ref. [37] that developed a Mixed-Integer-Linear-Programming model to support logistic and processing decisions in the supply chain, they applied their model in case study in Spain. Further [38], studied the effect of the variations on availability of raw material and product demands through a model to determine the optimal supply chain for lignocellulosic biomass. On the other hand [39], presented a new optimization approach to determine the water-energy-food nexus in a food supply chain accounting economic, environmental and sustainability criteria simultaneously. Finally, to solve bi-objective models [40], developed a new algorithm to solve bi-objective models using pairwise comparisons [40]. applied their methodology to optimize feedstock mix at a biomass fed district heating plant in Canada.

Because of the nature of the problem, thermodynamic packages are not really required, although in necessary case the adequate equations should be provided. Nevertheless, even feasible solutions of resulting models can extremely be hard to obtain.

Besides, most of resulting mathematical models for supply chain planning are Mixed Integer Linear Programming (MILP) problems, this type of problems can be solved using algebraic modelling languages such as GAMS, AMPL, LINGO, Pyomo or JUMP. These software allow solve complex mathematical formulations using special solvers for optimization (CPLEX, BARON, DICOPT, IPOPT, GUROBI, etc). Table 2 summarizes the problem type, used software, solvers and objectives for different supply chain types addressing the planning problem reported in literature as well as the comparison with the current paper.

### 2.4. Sustainability criteria and supply chain assessing

It is essential to mention that supply chains can be evaluated via several sustainability dimensions. In this regard, sustainability criteria involve economic, environmental and social aspects, as well as the interactions of them over time. These dimensions have been included in several papers; for example [41], included some sustainability criteria in a mathematical model for planning an ethanol supply chain. More recently [42], considered social, economic and environmental dimensions in a case study for an energy water supply chain in Mexico.

**Table 3**
Literature review regarding biomass, water and biofuels supply chains considering economic, environmental and social objectives.

| Supply chain type | Authors | Ref | Economic | | | | Environmental | | | | Social | | | | GIS | Additional comments |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | Net profit | Net present value | Cost | Minimum Sustainable Price | Impact indicator | GHGE | Water consumption | Others | Jobs | Social Opportunity | Social responsibility | Marginalization level | | |
| Cellulosic biofuels supply chains | You et al. (2012) | [41] | | X | | | | X | | | X | | | | | |
| Water supply chain | Fuentes-Cortés et al. (2019) | [42] | | | X | | | X | X | | X | X | | | | |
| Biomass supply chain | Santibañez-Aguilar et al. (2019a) | [44] | X | | | | | | | | | | | | X | |
| Bioethanol supply chain | Rahemi et al. (2020) | [45] | | | X | | | | | | | | | | X | Include a measure for suitability |
| Photovoltaic supply chain | Goodrich at al. (2013) | [46] | | | | X | | | | | | | | | | |
| Biomass supply chain | Ferro et al. (2018) | [47] | | X | | | | | | | | | | | | |
| Biofuels supply chain | Santibañez-Aguilar et al. (2011) | [48] | X | | | | X | | | | | | | | | |
| Chemical supply chain | Azapagic and Clift (1999) | [51] | | | X | | | | | X | | | | | | Consider the production level |
| Perfume Industry | Martinez-Guido et al. (2014) | [49] | X | | | | X | | | | | | | | | |
| Biofuels supply chain | Santibañez-Aguilar et al. (2014) | [50] | X | | | | X | | | | X | | | | | |
| Biofuels and fossil fuels supply chain | Sánchez-Bautista et al. (2017) | [6] | X | | | | | X | | | X | | | | | |
| Biofuels supply chain | Ahmed and Sarkar (2019) | [5] | | | X | | | X | | | X | | | | | |
| Bioethanol supply chain | Ghaderi et al. (2018) | [43] | | | X | | X | | | | | | X | | | |
| Biomass supply chain | Santibañez-Aguilar et al. (2019b) | [67] | X | | | | | | | | | | | | X | Consider the suitability and satisfaction level |
| Bioethanol supply chain | Ahranjani et al. (2018) | [52] | | | X | | | X | | | X | | | | | Consider uncertainty in supply chain |
| Energy and water supply chain | Cansino-Loaeza et al. (2018) | [53] | | | X | | | X | X | | | | | X | | Marginalization index is not used as objective |
| Bioenergy and biofuel supply chain | Akhtari and Sowlati, (2020) | [31] | | X | | | | | | | | | | | | |
| Bioethanol supply chain | Gilani et al. (2020) | [32] | X | | | | | | | X | | | | | | Profit is expected, social performance |
| Biogas supply chain | Diaz-Trujillo and Nápoles-Rivera, (2019) | [25] | X | | | | | | | | | | | | | |

(continued on next page)

**Table 3** (*continued*)

| Supply chain type | Authors | Ref | Economic | | | | Environmental | | | | Social | | | | GIS | Additional comments |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | Net profit | Net present value | Cost | Minimum Sustainable Price | Impact indicator | GHGE | Water consumption | Others | Jobs | Social Opportunity | Social responsibility | Marginalization level | | |
| Biogas supply chain | Durmaz and Bilgen, (2020) | [4] | X | | | | | | | | | | | | | Distance between facilities |
| Biomass Supply chain | Espinoza-Vázquez et al. (2020) | [38] | X | | | | | | | | | | | | | Product demand |
| Biomass to power supply chain | Fattahi et al. (2020) | [26] | X | | | | | | | | | | | | | |
| Food supply chain | Martinez-Guido et al. (2019a) | [39] | | | X | | | | | | | | | | | Human development index only is evaluated |
| Algal biomass to biodiesel supply chain | Yadala et al. (2020) | [36] | X | | | | | | | | | | | | | |
| Biomass to power supply chain | Yahya et al. (2021) | [28] | X | | | | | | | | | | | | | |
| Cellulosic biofuel supply chain | Ge et al. (2021) | [35] | X | | | | | | | | | | | | | |
| Biomass supply chain | This paper | | X | | | | | X | | | | | | X | | Consider social impact location |

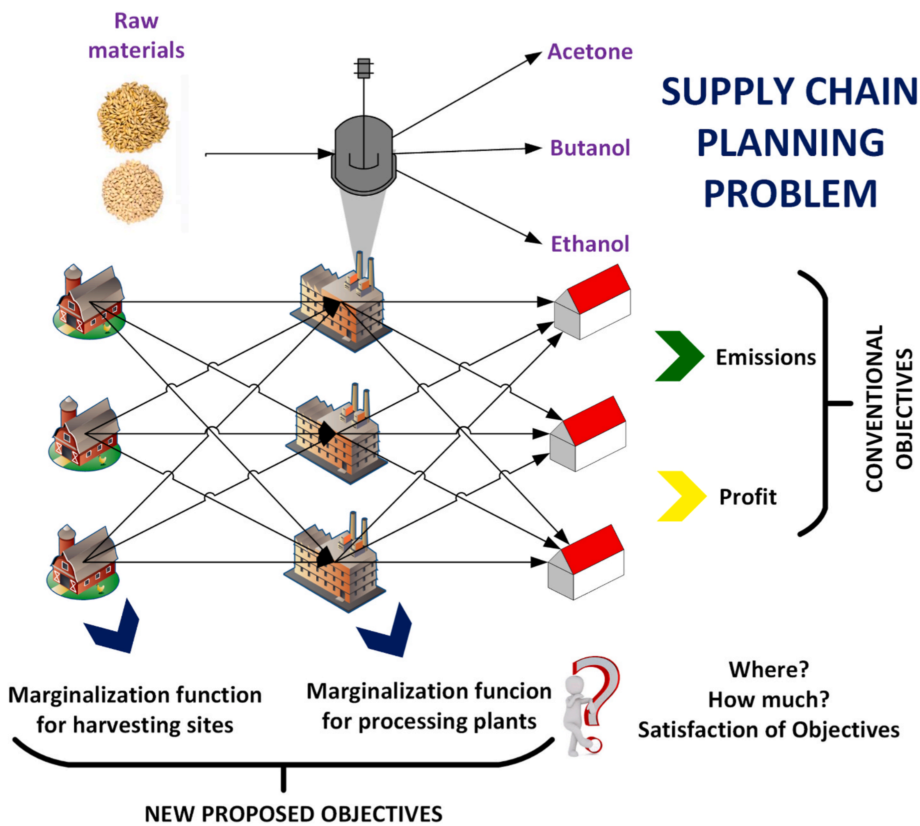


**Fig. 1.** Proposed superstructure for the addressed problem regarding an ABE process supply chain considering social functions based on marginalization index as well as economic and environmental objective functions.

Also [5], presented a multi-objective model for a biofuels supply chains considering the total cost as economic objective, carbon emission as environmental objective and created jobs as social objective [43]. developed a programming model for the sustainable design of a bio-ethanol supply chain considering economic, environmental and social objectives.

Economic dimension has been widely addressed in the literature and several authors have included this issue in their works via different variables such as the net annual profit, manufacturing cost, net present value, internal return rate or minimum sustainable price. For instance Ref. [44], considered the net annual profit for the planning of a multi-product supply chain based on residual biomass, they combined the model with a Geographic Information System approach. Also [45], formulated a bi-objective mixed-integer linear programming (MILP) model for the planning of a bioethanol supply chain considering competition of food and biomass feedstocks over the available crop-lands, such model considered the minimization of the cost and maxi-mization of the suitability simultaneously. It is important to note that [45] involved GIS into the evaluation of land suitability [46]. proposed an economic model to assess photovoltaic manufacturing systems through a parameter known as minimum sustainable price. Additionally [47], used the net present value as objective function for an optimization model based on power production from biomass. Also, the net profit has been considered as economic objective by Refs. [6,48–50].

Regarding to the environmental impact it has also been considered through diverse metrics such as Carbon footprint, Water consumption, Greenhouse gas emissions, Eco-Indicator99 or Eco-Efficiency Index. For example [48], included the environmental impact through the Eco-Indicator99 in a biomass processing system considering the Life-Cycle-Analysis. Also [51], took into account several objective functions in a multi-objective problem [49]. presented a multi-objective approach for the ambrox® production considering the environmental impact based on the Eco-indicator99 methodology [6]. proposed a multi-objective model for the biofuel and fossil fuels supply chain considering the greenhouse gas emissions as environmental objective [5]. developed a research to design a sustainable supply chain frame-work minimizing the total carbon emissions as environmental objective, as well as social and economic issues. In addition [52], considered the greenhouse emissions as environmental objective in a supply chain for a bioethanol production.

In contrast, social impact has been addressed in few works because historically, the social issue has been difficult to be considered. For that reason, most of them have not evaluated the social aspect when supply chain planning problem is addressed. In this sense [41], presented an optimal planning approach for ethanol production considering envi-ronmental, economic and social objectives. Moreover [5,6,50], used the generated jobs to evaluate new supply chains based on biomass pro-cessing. However, an objective based on jobs can easily get wrong in-terpretations. Hence, generated jobs present certain weakness such as social objective; for instance, if a supply chain topology represents a large number of new jobs, the social objective is not necessary a good value. An adequate social objective perhaps should indicate the location, where jobs take place.

An alternative to evaluate the social impact could be the marginal-ization index (MI), which is a multifactorial parameter that is related with the social deprivation. Also, MI allows identifying locations without basic services for human communities. Regarding the margin-alization index to evaluate processing systems [53], used the margin-alization index to define their case in a margined state in Mexico, but they did not use the marginalization index to evaluate their solution. Even though [22] presented a more robust manner to obtain a margin-alization index for Canada, they did not propose functions to evaluate any system based on the marginalization index. It is worth noting that despite advantages of marginalization index over other measures, there are not approaches with marginalization index formally included in the social impact evaluation for production system.

In conclusion, optimal supply chain planning is not a novel problem where economic, environmental and social objectives have been considered since we can observe papers from 2011 to 2020. In this context, there is a variety of ways to consider economic and environmental aspects properly. Nevertheless, most of the works have considered the social impact through generated jobs, which could not be the best manner to consider the social objective. To evaluate the social impact is required a multifactorial indicator. In fact, there is a lack of papers that considered a social indicator to assess the social impact. For instance Refs. [42,43], considered the social impact by a multifactorial objective such as social responsibility and social opportunity, although these may not be enough.

Therefore, to contribute to the state of the art concerns the supply evaluation though social criteria, this work presents a mathematical approach for the optimal planning of a supply chain considering a social objective function based on the marginalization index (MI) because marginalization index is a multifactorial index that is expressed as lack of opportunities and differences in economic resources for certain social communities, which affects the development of these communities. Table 3 illustrates the main differences between papers discussed in literature review regards supply chain assessing as well as this paper.

## 3. Problem statement

Fig. 1 presents a schematic representation for the proposed approach in current paper. Production system considers the production of acetone, butanol and ethanol via the ABE process using biomass. Hence, biomass can be obtained from several harvesting sites and processed into different facilities. Consequently, the obtained product can be delivered to consumers. In this sense, our approach consists in a mathematical model for the optimal planning of a supply chain focused on the ABE process, which considers the three main sustainability dimensions. Regarding the economic dimension, the model considers the net annual profit. The second one is the environmental impact measured via the net emissions caused by the new supply chain installation. Additionally, the social dimension is considered via two objective functions based on the marginalization index. It is worth noting that these objective functions promote that supply chain facilities (harvesting sites and processing plants) to be installed in marginalized communities in order to contribute to their social development.

The addressed problem can be formally defined as follows:

Given:

- Availability data for different raw materials.
- Conversion data for each raw material and processing route based on ABE technology.
- Demand data for acetone, butanol and ethanol in different consumption regions.
- Data to obtain the processing cost for ABE process.
- Data for marginalization index for different sites proposed as potential supply chain locations.
- Processing capacity limits according to different technologies.
- Data for emissions with respect to transportation, production and processing of raw material and products.
- Data for product prices and raw material costs.
- Distance between the potential supply chain facilities.

To obtain.

- Supply chain topologies under different economic, environmental and social conditions.
- Amounts of used raw material and produced products.
- Tradeoffs between social, economic and environmental objectives.

## 4. Mathematical model

The mathematical model section is divided in two sections. The first one presents the mathematical model assumptions while second one describes the considered equations.

### 4.1. Mathematical model assumptions

Main assumptions for the mathematical model are described as follows:

- The mathematical model considers constant parameters for the mass balances and economic functions. It is a deterministic approach.
- The reactor can process different types of raw materials with different cellulose compositions.
- Relationships for conversion of raw materials to products are assumed to be constant in a black box model. Although, these relationships can be obtained via ASPEN plus simulations or experimental information.
- Raw material processing is like a black box to obtain a linear function between produced product and used raw material.
- Amount of produced product is highly dependent on cellulose amount contained in raw material.
- Transportation function costs are linear with the distance as parameter and the transported material as variable.
- Function of capital investment is linearized as function of production capacity. Although rigorously, this function should be nonlinear
- Social impact is based on marginalization index to analyze the effect of the supply chain facility locations.

### 4.2. Considered equations

Most of constraint are based on macroscopic mass balances of raw material and products between supply chain facilities. Also, functions to compute the capital investment and associated cost are included. In addition, equations associated to $CO_2$ emissions caused by transportation, processing and raw material production are considered. Finally, several objective functions that allow defining the final topology of the supply chain. The proposed mathematical model consists of the following relationships.

#### 4.2.1. Raw material availability in biomass suppliers

It should be noticed that raw materials are not unlimited, for this reason, it is necessary to limit the raw materials to be used in production system. This way, the used raw material should be lower than the maximum available biomass. In addition, if any raw material is used, the amount of raw material should be greater than a lower limit to satisfy a feasibility transportation constraint. To satisfy lower and upper limits, the implemented mathematical model considers a binary variable to define if raw material is used, therefore, if raw material is fed, then the binary variable should be equal to 1, whereas if raw material is not used, then the binary variable is equal to zero.

$$F_{m,s}^{used} \leq F_{m,s}^{\max} \cdot y_{m,s}^{used}, \quad \forall m \in RawMaterials, s \in Suppliers \tag{1}$$

$$F_{m,s}^{used} \geq F_{m,s}^{\min} \cdot y_{m,s}^{used}, \quad \forall m \in RawMaterials, s \in Suppliers \tag{2}$$

#### 4.2.2. Raw material distribution from biomass suppliers to plants (reactors)

Each processing plant is associated to a reactor or process technology. In this regard, the amount of used biomass is equal to the sum of distributed biomass from harvesting sites to processing facilities.

$$F_{m,s}^{used} = \sum_{r} F_{m,s,r}^{S-R}, \quad \forall m \in RawMaterials, s \in Suppliers \tag{3}$$

#### 4.2.3. Received raw material from diverse biomass suppliers

Additionally, the total received biomass is equal to the sum of distributed raw material between harvesting sites to processing plants. It should be noted that the proposed mathematical formulation takes into account that each processing plant has a cellulose rector to be used in the ABE processing routes.

$$F^{R}_{m,r} = \sum_{s} F^{S-R}_{m,s,r}, \quad \forall m \in RawMaterials, r \in Plants \tag{4}$$

### 4.3. Balance for cellulose in reactor's feed

Furthermore, the processing of raw materials is modelled through cellulose reactors in processing plants. It is worth noting that each reactor can receive multiples feedstocks with different cellulose compositions. Hence, the cellulose amount should be obtained, then, the cellulose amount received in any reactor is equal to the total flow received in the reactor multiplied by the cellulose fraction, which is equal to the sum of cellulose amounts for each feedstock.

$$F^{feed}_{r} \cdot x^{cel}_{r} = \sum_{m} \left( F^{R}_{m,r} \cdot x^{R}_{m,r} \right), \quad \forall r \in Plants \tag{5}$$

It is worth noting that a Mixed Integer Linear Programming (MILP) problem is much easier to solve than a Mixed Integer Non-Linear Programming (MINLP) model. In addition, a MILP formulation allows obtaining a global optimal solution. Nevertheless, the main limitation of our formulation is Equation (5), which considers the cellulose balance in reactors. It should be noted that cellulose fraction in each raw material is different and it can be a parameter into the model. In contrast, the cellulose fraction in reactors depends on the previous fraction which is unknown since amount received in each reactor for each biomass type is determined by the solver. In this way, Equation (5) considers a multiplication for variables (cellulose fraction in reactor and received raw material). In summary:

$x^{cel}_{r}$ Variable.
$F^{feed}_{r}$ Variable.
$F^{R}_{m,r}$ Variable.
$x^{R}_{m,r}$ Parameter.

### 4.4. Total mass in the reactor's inlet

In addition, the total amount of biomass at the reactor's inlet is equal to the sum of all feedstocks for each raw material.

$$F^{feed}_{r} = \sum_{m} \left( F^{R}_{m,r} \right), \quad \forall r \in Plants \tag{6}$$

### 4.5. Flowrate in reactor's outlet

The produced product amount depends on the cellulose amount. This way, the obtained product is equal to the cellulose amount in the processing plant multiplied by a conversion factor, which represents the amount of produced product per cellulose amount.

$$F^{P}_{r,p} = \alpha^{cell-P}_{r,p} \cdot \sum_{m} \left( F^{R}_{m,r} \cdot x^{R}_{m,r} \right), \quad \forall r \in Plants, p \in Products \tag{7}$$

It is important to mention that the flowrate depends on the conversion factor for each reactor and the conversion factor can be different for several types of technologies. For instance, ABE technologies with different acetone, butanol and ethanol proportion.

### 4.6. Product distribution to different consumption regions

An important supply chain stage is the product distribution to the consumption regions; then, the obtained product is equal to the sum of distributed products from processing sites to consumption regions.

$$F^{P}_{r,p} = \sum_{c} F^{R-C}_{r,p,c}, \quad \forall r \in Plants, p \in Products \tag{8}$$

### 4.7. Received product from plants (reactors)

The product amount in each consumption region is equal to the sum of the distributed product from processing plants.

$$F^{C}_{c,p} = \sum_{r} F^{R-C}_{r,p,c}, \quad \forall c \in ConsumptionRegion, p \in Products \tag{9}$$

### 4.8. Demand product in consumption region

In addition, the proposed mathematical model includes a constraint to limit the product amount to be delivered in consumption regions. Equation (10) states that delivered product amount should be lower than the required demand for each product and consumption region.

$$F^{C}_{c,p} \le F^{Demand}_{c,p}, \quad \forall c \in ConsumptionRegion, p \in Products \tag{10}$$

### 4.9. Transportation costs and emissions

The transportation cost is also considered, which depends on the distance between the nodes in which product or biomass is transported as well as the amount of material to be distributed. It should be noted that transportation cost equation considers the transportation cost for biomass between harvesting sites and processing plants and, the transportation cost for products from processing facilities to consumers.

$$TC = \sum_{m}\sum_{s}\sum_{r} C^{transp-M}_{m} \cdot F^{S-R}_{m,s,r} \cdot d^{S-R}_{s,r} + \sum_{p}\sum_{r}\sum_{c} C^{transp-P}_{p} \cdot F^{R-C}_{r,p,c} \cdot d^{R-C}_{r,c} \tag{11}$$

Furthermore, the environmental impact is a crucial issue that should be considered in the supply chains design. For that reason, the mathematical approach accounts for the environmental impact for transportation between harvesting sites and processing facilities, as well as processing sites and consumption region. This equation is similar to the Equation for transportation costs (Eq. (11)).

$$TE = \sum_{m}\sum_{s}\sum_{r} E^{transp-M}_{m} \cdot F^{S-R}_{m,s,r} \cdot d^{S-R}_{s,r} + \sum_{p}\sum_{r}\sum_{c} E^{transp-P}_{p} \cdot F^{R-C}_{r,p,c} \cdot d^{R-C}_{r,c} \tag{12}$$

### 4.10. Operating cost and processing emissions

In addition, operating cost and environmental impact are modelled as function of the raw material amount (cellulose). Therefore, total operating cost and environmental impact are calculated via a unitary operating cost and environmental impact as well as the cellulose amount fed to each processing facility.

$$OC = \sum_{r} C^{operating}_{r} \cdot \left( \sum_{m} \left( F^{R}_{m,r} \cdot x^{R}_{m,r} \right) \right) \tag{13}$$

$$OE = \sum_{r} E^{operating}_{r} \cdot \left( \sum_{m} \left( F^{R}_{m,r} \cdot x^{R}_{m,r} \right) \right) \tag{14}$$

### 4.11. Capital investment

Besides, the proposed mathematical formulation considers an Equation to calculate the capital investment. It should be noted that the capital investment depends on the processing capacity. Additionally, the model uses a factor KF to account the depreciation cost associated to the capital investment in order to be included in the net annual profit function.

$$CC = KF \cdot \sum_{r}\sum_{q} \left[ A_{r,q} \cdot y^{cap}_{r,q} + B_{r,q} \cdot \left( F^{capq}_{r,q} \right) \right] \tag{15}$$

It is worth noting that the proposed capital cost function is a linear function that depends on diverse intervals for the processing capacity. Where the processing capacity is a variable; which limits the amount of processed raw material.

$$F_r^{cap} \geq F_r^{feed}, \quad \forall r \in Plants \tag{16}$$

Furthermore, the full process capacity is equal to the sum of process capacity for each interval.

$$F_r^{cap} = \sum_q F_{r,q}^{capq}, \quad \forall r \in Plants \tag{17}$$

It is important to note that only one interval for process capacity is selected. For that reason, the discretized processing capacity is associated to a binary variable. This binary variable is equal to 1 if the discretized processing capacity is an amount limited by upper and lower bounds for each interval. Additionally, constraint (20) ensures that only one interval is selected.

$$F_{r,q}^{MAX-cap} \cdot y_{r,q}^{cap} \geq F_{r,q}^{capq}, \quad \forall r \in Plants, q \in IntervalCapacity \tag{18}$$

$$F_{r,q}^{MIN-cap} \cdot y_{r,q}^{cap} \leq F_{r,q}^{capq}, \quad \forall r \in Plants, q \in IntervalCapacity \tag{19}$$

$$\sum_q y_{r,q}^{cap} = 1, \quad \forall r \in Plants \tag{20}$$

### 4.12. Revenue for selling of products

One of the objectives of the butanol, ethanol and acetone productions is their commercialization. In this sense, the revenue of sold products is equal to the sum of a unitary product price multiplied by the total produced product.

$$RP = \sum_c \sum_p C_{c,p}^{product} \cdot F_{c,p}^C \tag{21}$$

### 4.13. Emissions associated to use products

Besides, the use of products is associated to an environmental impact. This environmental impact depends on the amount of yielded product as well as a unitary value for environmental impact. It is worth nothing that the environmental coefficient is strongly related with the use of products because the unitary impact is different if the products are fuels, chemicals, or raw materials for future processes.

$$EP = \sum_c \sum_p E_p^{product} \cdot F_{c,p}^C \tag{22}$$

### 4.14. Biomass production cost

Also, the proposed mathematical model considers the biomass production cost, this cost is equal to a unitary biomass cost multiplied by the amount of produced biomass. It should be noted that the biomass production cost is associated to each harvesting site.

$$BC = \sum_m \sum_s C_{m,s}^{biomass} \cdot F_{m,s}^{used} \tag{23}$$

### 4.15. Emissions associated to biomass production

Similarly, the emissions associated to the biomass production must be calculated; in this sense, the total biomass production emissions are equal to a unitary emission factor multiplied by the amount of produced biomass in each biomass supplier.

$$BE = \sum_m \sum_s E_m^{biomass} \cdot F_{m,s}^{used} \tag{24}$$

### 4.16. Net annual profit

Additionally, the net annual profit is calculated through the previously mentioned economic terms (revenue, operating cost, capital cost and transportation cost) as follows:

$$NetProfit = RP - BC - CC - OC - TC \tag{25}$$

### 4.17. Net emissions

On the other hand, the net emissions are obtained from the sum of emissions for biomass production, product use, processing plant operation and transportation.

$$NetEmission = BE + EP + OE + TE \tag{26}$$

### 4.18. Social objective functions

It is worth noting that the social aspect is a crucial issue that should be considered in any supply chain design methodology. Nevertheless, the most of works have not included the social aspect as a formal objective function. This index can be estimated by government institutions and it strongly depends on locations, since each location has different quality of life.

In case of Mexico, the marginalization index is reported by National Council of Population (CONAPO) and considers at least 9 factors related with the development level of the community (see Table 1). The main characteristic of the marginalization index to be used for mathematical model in this paper is that marginalization index depends over location and therefore an adequate mathematical function can be used to promote the selection of marginalized locations when the supply chain planning problem is solved since installation of supply chain facilities in marginalized locations can enhance the life quality of communities.

As commented, marginalization index considers several features to obtain the marginalization level for diverse locations. Social objective function in this model is expressed in terms of binary variables to obtain the overall margination level based on the selected locations for the supply chain.

It is worth noting that current research considers the social impact through a social objective function. This objective function depends on the location of processing plants and harvesting sites. It should be noticed that contribution to the social impact is different for processing plants and harvesting sites and then a processing plant in location A has a different social impact that a harvesting site in location A. At this point, it is crucial to remember that social impact is related with location, potential harvesting sites are commonly located in rural regions, while potential processing plants are commonly located in urban regions.

First term of social objective function is the overall non-margination level for the use of raw material from harvesting sites. Hence, if a location X is selected for the supply chain (a raw material is selected from a specific harvesting site), then, the unitary margination index for location X contributes to the overall social function; otherwise, the effect over the social objective function is zero. Binary variables for biomass suppliers' location are linked with the amount of used raw material.

$$Term^{harvesting} = \left(\frac{1}{TotalRawMaterials}\right) \sum_s \sum_m F_s^{Margin-harvesting} \frac{y_{s,m}^{used}}{TotalSites} \tag{27}$$

Second term of social objective function is associated to the processing facility locations installations in the potential locations. Here, binary variables for processing facility locations are linked with the amount of processed biomass in the processing plants. In other words, if a processing plant is chosen into the supply chain design, then the binary variable associated to that process facility is equal to 1, otherwise, this binary variable is equal to zero.

$$Term^{plants} = \sum_{r}\sum_{q} F_{r}^{Margin-plants} \frac{y_{r,q}^{cap}}{TotalPlants} \quad (28)$$

Social impact is considered into a single objective, which considers the sum of two social terms (see Equations (27) and (28)). It should be noticed that term associated to harvesting facilities is divided between the number of total raw materials to weight adequately the terms because the processing facilities term does not depend of the raw materials.

$$SocialObjective = Term^{harvesting} + Term^{plants} \quad (29)$$

### 4.19. Nature of constraints

As can be seen, constraints in mathematical model can be divided in linear inequalities, linear equations and nonlinear equations. In summary, the linear inequalities correspond to equations ((1), (2), (10), (16), (18) and (19). Linear equations are depicted by equations (((3), (4), (6)–(9), (11)–(15), (17), (20)–(29). Finally, the non-linear Equation is Equation (5).

Further, equations ((1) and (2) and (15) and (18)–(20) and (27) and (28) contain binary variables into the formulation. Based on this, it is possible to conclude that mathematical formulation is a Mixed Integer Non-Linear Programming model.

## 5. Solution approach

The presented formulation is a Mixed Integer Non-Linear Programming (MINLP) Problem and the model has taken into account four objectives for the ABE production system planning. Therefore, a multi-objective algorithm should be used to find the tradeoff between objectives.

There are different alternatives to solve multi-objective problems, which could be classified in generators methods and based on preference. The main advantage of the methods generators is that it is possible to generate information for multiple solutions but, it implies more computational resources. In contrast, event though, based on preference methods allow reduce the computational resources, the obtained solution could be slanted to the preference provided when method is applied. Both alternatives are based on formulating of a multi-objective problem into one or several single objective problems.

Additionally, there are alternatives focused on multi-objective problems considering uncertainty. For instance Ref. [54], presented an algorithm very useful for a system under uncertainty and some parameters could be unknown, in which, some parameters would need a probability distribution. Also, method used by Ref. [55] implies to formulate the multi-objective problem into a single objective problem through different weights for the objective functions based on experience level.

[56] used a multi-stakeholder decision-making approach to balances the dissatisfaction of different stakeholders for a optimization problem with five objectives; the justification was that a final decision-maker would need to select a solution point from the Pareto set and this selection might not be obvious. The presented strategy for [56] is powerful and useful when decision makers want to avoid the generation of the complete Pareto set. A similar strategy has been used by Ref. [57], in which a multi-objective optimization problem was formulated into a single objective problem based on a compromise solution objective function.

As mentioned, there are generator methods and based on preference to solve multi-objective problems. One of the most used generator methods is known as epsilon-constraint, which its main objective is to generate multiple solutions to provide information and to obtain the Pareto sets between objectives, this method can be applied to any number of objectives, but generated Pareto curve is not easy to visualize when objectives are greater than two or three. Epsilon-constraint method is an efficient method to solve multi-objective problems in which an objective is chosen to be optimized; while the other objectives are formulated as constraints and Pareto fronts could be generated [58].

In this paper, the epsilon-constraint method was used to generate several Pareto curves with two objectives each one to illustrate the tradeoff between the involved objectives. Even though this pairwise objective analysis could not be practical, it is possible to generate enough information to stakeholders to observe the behavior and relationships between objectives. Additionally, planning problems are solved for long time horizons and then, extra computational resources and time by solution generation and analysis are not too relevant. Combinations to generate Pareto curves are listed as follows:

- Net annual profit and Environmental impact
- Net annual profit and Social Objective
- Environmental impact and Social objective

As mentioned, paper is focused on the supply chain planning of the ABE process using methodologies based on mathematical programming. This type of approaches could be solved using different software such as GAMS, AMPL, LINGO, PYOMO, JUMP or even MATLAB, the reason why others commercial software or codes like PHP, Visual Basic, MS-Excel or ASPEN plus are not used is because some types of constraints (inequalities) and variables (binary variables) are not easy to implement.

Nevertheless, commercial simulators could be used by combination with algebraic modelling languages if required. For example [59], used model for the Gibbs free energy minimization to determine the species distribution when the reaction system reaches the equilibrium at different reaction conditions in a process for polycrystalline silicon production [59]. used GAMS to solve the Non-Linear Programming problem due to Gibbs free energy minimization model, while used ASPEN plus for the rigorous modelling and sizing of the separation system based on distillation columns.

In this regard, a supply chain planning approach could use ASPEN plus to model the reaction system to obtain reaction conditions, molar conversion, recommended equipment size, etc. Subsequently, it might use an algebraic modelling language to solve the planning problem. Specifically, in this paper only the planning problem is addressed while the processing data are obtained offline.

## 6. Case study

We applied our mathematical model to a hypothetical case study in Mexico. It should be noticed that a supply chain analysis depends strongly over the case study scale. Some essential aspects to decide the scale of the problem are the size of the problem and the accuracy. In this respect, a small scale works better for functions like transportation, processing and it can be applied to more realistic cases. For instance, a processing plant can be located in a municipality and it can receive raw material from a near municipality, then the associated transportation costs could be more accurate than in a bigger scale. However, the computational resources to solve the supply chain could increase dramatically. On the other hand, if a full country is divided in bigger sections, the transportation costs probably would be poorly computed, although the computational resources would be so lower.

Particularly, Mexico has around 2400 municipalities and the solution for 2400 potential locations could be considered so much complex if a previous pre-selection of candidates like accomplished by Refs. [60,61] or [4] is not considered. For that reason, a study at municipal level only could be applied to a low number of municipalities like [25,39]. In this respect, Federal states is an adequate level for a study if the objective is to show a general supply chain in National context, some examples are research by Refs. [30,38].

Furthermore, another aspect that affects the selection of potential

**Table 4**
Raw material availability for each potential location (Mg/year) [62].

| Names (Raw Material/Suppliers) | ID | Wheat straw 1 | Sugar cane 2 | Wheat 3 | Corn grain 4 | Sorghum grain 5 | Cassava root 6 | Sugar beet 7 | Sweet sorghum 8 |
|---|---|---|---|---|---|---|---|---|---|
| Aguascalientes | 1 | 252 | – | 140 | 64,271 | 64,271 | 41 | 140 | 14 |
| Baja California | 2 | 3,925,838 | 0 | 2,181,021 | 1086 | 8151 | 41 | 140 | 140 |
| Baja California Sur | 3 | 50,400 | 3 | 28,000 | 31,702 | 3265 | 41 | 140 | 140 |
| Campeche | 4 | 252 | 695,222 | 140 | 420,551 | 51,913 | 41 | 5600 | 5600 |
| Coahuila | 5 | 10,080 | – | 5600 | 43,560 | 9474 | 41 | 140 | 140 |
| Colima | 6 | 252 | 1,459,085 | 140 | 48,430 | 8607 | 41 | 140 | 140 |
| Chiapas | 7 | 252 | 2,854,599 | 140 | 1,188,400 | 42,549 | 41 | 5600 | 140 |
| Chihuahua | 8 | 50,400 | – | 28,000 | 1,373,410 | 38,490 | 41 | 5600 | 140 |
| Distrito Federal | 9 | 252 | – | 140 | 5400 | 0 | 41 | 140 | 140 |
| Durango | 10 | 10,080 | – | 5600 | 413,212 | 22,376 | 41 | 5600 | 5600 |
| Guanajuato | 11 | 10,080 | 74 | 5600 | 1,420,029 | 1,520,541 | 41 | 5600 | 140,160 |
| Guerrero | 12 | 252 | 1862 | 140 | 1,331,616 | 66,396 | 41 | 5600 | 5600 |
| Hidalgo | 13 | 252 | – | 140 | 650,898 | 669 | 41 | 140 | 140 |
| Jalisco | 14 | 252 | 7,560,123 | 140 | 3,497,303 | 295,730 | 41 | 140 | 5600 |
| México | 15 | 252 | 12,874 | 140 | 1,856,138 | 1166 | 41 | 140 | 140 |
| Michoacán | 16 | 252 | 1,727,035 | 140 | 1,935,287 | 757,039 | 41 | 140 | 5600 |
| Morelos | 17 | 252 | 2,027,620 | 140 | 84,152 | 187,566 | 41 | 140 | 140 |
| Nayarit | 18 | 252 | 2,429,420 | 140 | 195,496 | 295,815 | 41 | 140 | 5600 |
| Nuevo León | 19 | 50,400 | – | 28,000 | 82,839 | – | 41 | 140 | 5600 |
| Oaxaca | 20 | 10,080 | 4,146,059 | 5600 | 646,851 | – | 41 | 5600 | 140,160 |
| Puebla | 21 | 252 | 1,602,869 | 140 | 960,406 | – | 41 | 140 | 140 |
| Querétaro | 22 | 252 | – | 140 | 284,778 | – | 41 | 140 | 140 |
| Quintana Roo | 23 | 252 | 1,552,033 | 140 | 49,417 | – | 41 | 5600 | 5600 |
| San Luis Potosí | 24 | 252 | 5,041,240 | 140 | 192,280 | – | 41 | 5600 | 140 |
| Sinaloa | 25 | 252 | 818,633 | 140 | 3,686,587 | – | 41 | 28,000 | 140,160 |
| Sonora | 26 | 252,288 | – | 140,160 | 135,507 | – | 41 | 140 | 5600 |
| Tabasco | 27 | 252 | 2,211,117 | 140 | 129,608 | – | 41 | 5600 | 140 |
| Tamaulipas | 28 | 252 | 3,520,279 | 140 | 527,056 | – | 41 | 140 | 140,160 |
| Tlaxcala | 29 | 252 | – | 140 | 364,450 | – | 41 | 140 | 140 |
| Veracruz | 30 | 252 | 19,193,277 | 140 | 1,264,855 | – | 41 | 5600 | 140 |
| Yucatán | 31 | 252 | 570 | 140 | 105,724 | – | 41 | 140 | 140 |
| Zacatecas | 32 | 10,080 | 7140 | 5600 | 335,536 | – | 41 | 140,160 | 140 |

supply chain facilities is the data availability. Specially, Mexico has various public databases generated by Mexican government agencies; which provide information regarding production of agricultural crops and their prices (SADER-Ministry of Agricultural and Rural Development), development level of population (INEGI-National Institute for Statistic, Geographic and Informatic), infrastructure for transportation (SCT-Ministry of Transportation and Communications), marginalization level of communities (CONAPO-National Council of Population) energy demand and fossil fuels resources (SENER-Ministry of Energy and PEMEX-Mexican Petroleum Company), even though some information need to be updated. In this sense most of information can be easily get at federal state scale.

Therefore, the case study addressed in this paper is defined at federal state level since it is an adequate level to provide the model in a National context and the more updated information can be also get at this level. Case study considers that each one of federal states as potential harvesting sites (they have available raw material), also 32 processing facilities (they could have production infrastructure) and 32 consumption regions (they have product demand) are contemplated. In summary, 1 harvesting site, 1 processing facility and 1 consumption region per each federal state.

Moreover, the addressed case study is focused in planning a supply chain for the ethanol, butanol and acetone production via the ABE process. Fortunately, several preliminary studies have been conducted in this regard. For example, taking as a base the agricultural availability presented in Refs. [19,48] presented a wide panorama associated to the yields in the fermentation process, as well as the costs associated with the necessary equipment and services.

On the other hand, the information regarding the equipment for the purification section has also been previously addressed by Refs. [20,21]. In their study, various separation schemes were presented considering a multi-objective approach. Thus, allowing to know some aspects associated with the economy and environmental impact of the process.

**Table 5**
Mass ratio between processed cellulose and produced product [19–21].

| Location | Mass ratio (Produced product/Used raw material) Acetone | Butanol | Ethanol | Operating cost ($US/Mg) |
|---|---|---|---|---|
| Aguascalientes | 4.6264 | 3.1058 | 0.7619 | 0.2030 |
| Baja California | 3.0223 | 3.5070 | 0.6820 | 0.3529 |
| Baja California Sur | 3.3911 | 5.7968 | 0.8726 | 0.3662 |
| Campeche | 6.0471 | 4.0813 | 0.9937 | 0.1521 |
| Coahuila | 6.7957 | 4.6164 | 1.1218 | 0.1376 |
| Colima | 4.0769 | 4.8323 | 0.8989 | 0.2541 |
| Chiapas | 5.3666 | 5.2213 | 1.0590 | 0.1794 |
| Chihuahua | 5.4848 | 4.8212 | 1.0403 | 0.1811 |
| Distrito Federal | 2.9735 | 4.6603 | 0.7376 | 0.4286 |
| Durango | 6.2813 | 4.2133 | 1.0327 | 0.1500 |
| Guanajuato | 3.8665 | 3.3818 | 0.7420 | 0.2498 |
| Guerrero | 2.9334 | 3.4807 | 0.6719 | 0.3765 |
| Hidalgo | 5.2838 | 4.4503 | 0.9786 | 0.1797 |
| Jalisco | 3.6528 | 5.6788 | 0.9037 | 0.3234 |
| México | 4.7008 | 5.3407 | 1.0053 | 0.2170 |
| Michoacán | 4.4956 | 5.4223 | 0.9894 | 0.2327 |
| Morelos | 6.5215 | 4.5975 | 1.0841 | 0.1411 |
| Nayarit | 5.6980 | 4.9238 | 1.0635 | 0.1669 |
| Nuevo León | 6.5851 | 4.7893 | 1.1298 | 0.1408 |
| Oaxaca | 4.1342 | 5.7339 | 0.9779 | 0.2744 |
| Puebla | 5.1366 | 5.0426 | 1.0280 | 0.1930 |
| Querétaro | 2.9506 | 4.8083 | 0.7436 | 0.3889 |
| Quintana Roo | 4.2929 | 4.7612 | 0.9166 | 0.2364 |
| San Luis Potosí | 3.2103 | 5.0614 | 0.8091 | 0.3713 |
| Sinaloa | 6.0449 | 4.8819 | 1.1038 | 0.1582 |
| Sonora | 3.8674 | 3.1210 | 0.7231 | 0.2535 |
| Tabasco | 5.2003 | 4.9881 | 1.0295 | 0.1979 |
| Tamaulipas | 3.8667 | 4.9085 | 0.8807 | 0.2799 |
| Tlaxcala | 5.3964 | 5.1834 | 1.0587 | 0.1793 |
| Veracruz | 3.7327 | 5.6324 | 0.9118 | 0.3406 |
| Yucatán | 3.1916 | 4.6432 | 0.7657 | 0.3849 |
| Zacatecas | 4.2809 | 4.6036 | 0.9066 | 0.2499 |

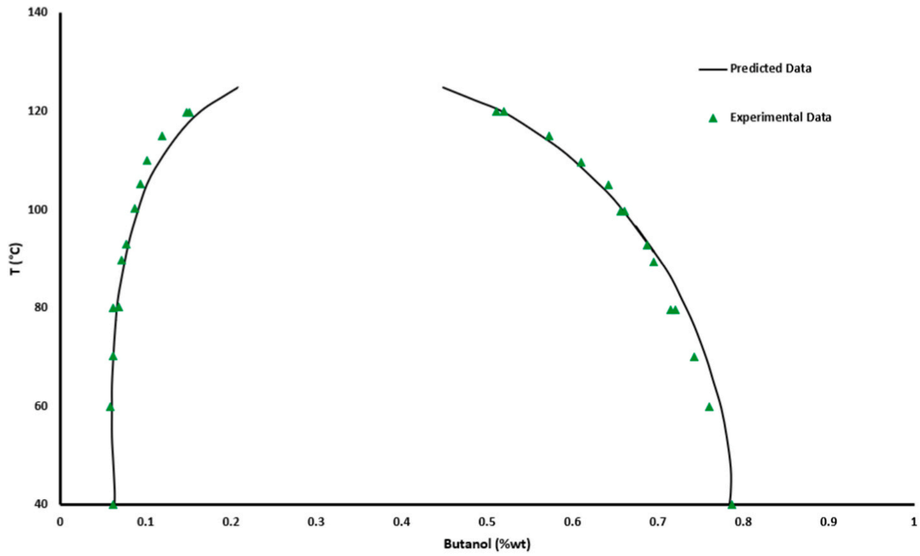


**Fig. 2.** Comparison between LLE predicted by NRTL model (line) and experimental data ([63]).

Note in both cases, through the implementation of the process intensification philosophy, it was possible to overcome the current conventional alternatives. The main improvement is clearly observed through the diminishment in total equipment performing the same operation. In the particular case of fermentation, the intensified reactor carried out saccharification and fermentation in the same equipment. Regarding process separation, the improvement was oriented in the same way. By means of a hybrid process followed by distillation columns with side stream or dividing wall columns, it was possible to overcome conventional technology measured through global energy requirements for ABE purification.

Concerning the materials, our case study considers 8 types of raw materials and 3 different products. Regarding the processing routes, we have considered three production intervals in order to include the dependence of the economies of scale. Potential supply chain locations, raw materials, products and routes are defined along this section.

Table 4 presents the raw material availability for each biomass supplier and biomass type. This raw material availability corresponds to the maximum biomass amount to be collected and processed.

Table 5 presents the mass ratio between the processed cellulose and

**Table 6**
Product demand and product price for each product and consumption region. (Estimated from gasoline demand, [66].

| Consumer | Product demand (Mg/year) | | | Product price ($US/Mg) | | |
|---|---|---|---|---|---|---|
| | Acetone | Butanol | Ethanol | Acetone | Butanol | Ethanol |
| Aguascalientes | 15,785,520 | 15,785,520 | 15,785,520 | 3000 | 1200 | 508 |
| Baja California | 36,956,688 | 36,956,688 | 36,956,688 | 3000 | 1200 | 508 |
| Baja California Sur | 8,635,608 | 8,635,608 | 8,635,608 | 3000 | 1200 | 508 |
| Campeche | 5,385,648 | 5,385,648 | 5,385,648 | 3000 | 1200 | 508 |
| Chiapas | 23,028,288 | 23,028,288 | 23,028,288 | 3000 | 1200 | 508 |
| Chihuahua | 34,263,864 | 34,263,864 | 34,263,864 | 3000 | 1200 | 508 |
| Coahuila | 17,456,928 | 17,456,928 | 17,456,928 | 3000 | 1200 | 508 |
| Colima | 23,214,000 | 23,214,000 | 23,214,000 | 3000 | 1200 | 508 |
| Distrito Federal | 114,491,448 | 114,491,448 | 114,491,448 | 3000 | 1200 | 508 |
| Durango | 22,006,872 | 22,006,872 | 22,006,872 | 3000 | 1200 | 508 |
| Guanajuato | 43,920,888 | 43,920,888 | 43,920,888 | 3000 | 1200 | 508 |
| Guerrero | 16,528,368 | 16,528,368 | 16,528,368 | 3000 | 1200 | 508 |
| Hidalgo | 36,585,264 | 36,585,264 | 36,585,264 | 3000 | 1200 | 508 |
| Jalisco | 52,370,784 | 52,370,784 | 52,370,784 | 3000 | 1200 | 508 |
| México | 60,449,256 | 60,449,256 | 60,449,256 | 3000 | 1200 | 508 |
| Michoacán | 36,585,264 | 36,585,264 | 36,585,264 | 3000 | 1200 | 508 |
| Morelos | 20,335,464 | 20,335,464 | 20,335,464 | 3000 | 1200 | 508 |
| Nayarit | 6,499,920 | 6,499,920 | 6,499,920 | 3000 | 1200 | 508 |
| Nuevo León | 68,992,008 | 68,992,008 | 68,992,008 | 3000 | 1200 | 508 |
| Oaxaca | 17,642,640 | 17,642,640 | 17,642,640 | 3000 | 1200 | 508 |
| Puebla | 42,620,904 | 42,620,904 | 42,620,904 | 3000 | 1200 | 508 |
| Querétaro | 24,699,696 | 24,699,696 | 24,699,696 | 3000 | 1200 | 508 |
| Quintana Roo | 0 | 0 | 0 | 3000 | 1200 | 508 |
| San Luis Potosi | 20,521,176 | 20,521,176 | 20,521,176 | 3000 | 1200 | 508 |
| Sinaloa | 26,092,536 | 26,092,536 | 26,092,536 | 3000 | 1200 | 508 |
| Sonora | 23,678,280 | 23,678,280 | 23,678,280 | 3000 | 1200 | 508 |
| Tabasco | 20,242,608 | 20,242,608 | 20,242,608 | 3000 | 1200 | 508 |
| Tamaulipas | 31,756,752 | 31,756,752 | 31,756,752 | 3000 | 1200 | 508 |
| Tlaxcala | 0 | 0 | 0 | 3000 | 1200 | 508 |
| Veracruz | 56,270,736 | 56,270,736 | 56,270,736 | 3000 | 1200 | 508 |
| Yucatán | 32,221,032 | 32,221,032 | 32,221,032 | 3000 | 1200 | 508 |
| Zacatecas | 8,449,896 | 8,449,896 | 8,449,896 | 3000 | 1200 | 508 |

**Table 7**
Data for capital cost for each processing technology [19–21].

| Processing plant | Variable term in capital cost function | | | Fixed term capital cost function | | |
|---|---|---|---|---|---|---|
| | (1000–10000) Mg/y | (10,000–25000) Mg/y | (25,000–50000) Mg/y | (1000–10000) Mg/y | (10,000–25000) Mg/y | (25,000–50000) Mg/y |
| | $US y/Mg | $US y/Mg | $US y/Mg | $US | $US | $US |
| Aguascalientes | 1.5062 | 2.7708 | 2.5513 | 3,479,106 | 4,268,142 | 7,015,968 |
| Baja California | 1.9845 | 3.7411 | 2.9819 | 3,049,187 | 5,487,136 | 4,553,817 |
| Baja California sur | 1.6540 | 1.9464 | 2.7711 | 2,900,638 | 5,746,042 | 5,826,673 |
| Campeche | 1.1371 | 1.9864 | 3.7183 | 2,805,398 | 4,169,443 | 4,793,415 |
| Chiapas | 1.0086 | 1.7334 | 5.4173 | 3,334,332 | 4,720,187 | 6,268,553 |
| Chihuahua | 1.4928 | 3.4707 | 1.6794 | 3,127,333 | 4,104,378 | 5,893,865 |
| Coahuila | 1.2077 | 1.6932 | 1.7485 | 3,335,181 | 4,570,878 | 5,722,882 |
| Colima | 1.1187 | 2.0199 | 1.9570 | 3,391,142 | 5,446,182 | 5,215,591 |
| Distrito Federal | 1.8180 | 3.4008 | 1.7503 | 3,317,412 | 4,536,429 | 5,677,653 |
| Durango | 1.1027 | 2.1722 | 2.4925 | 3,405,119 | 5,640,509 | 7,059,290 |
| Guanajuato | 1.6984 | 2.4228 | 2.0893 | 3,237,800 | 4,149,847 | 7,138,499 |
| Guerrero | 2.0099 | 3.1659 | 1.9926 | 2,519,370 | 3,837,554 | 6,921,273 |
| Hidalgo | 1.2617 | 3.5482 | 5.6397 | 3,025,731 | 4,279,321 | 5,173,004 |
| Jalisco | 1.5569 | 3.8251 | 1.9436 | 2,929,065 | 4,370,616 | 5,802,095 |
| México | 1.2878 | 3.2241 | 2.5691 | 2,825,650 | 4,071,815 | 6,381,482 |
| Michoacán | 1.3417 | 1.8114 | 2.0925 | 3,662,395 | 4,229,573 | 4,965,996 |
| Morelos | 1.0339 | 1.8470 | 1.7286 | 3,291,668 | 5,397,969 | 5,709,579 |
| Nayarit | 1.1186 | 2.5471 | 2.3953 | 3,180,408 | 4,213,426 | 5,653,399 |
| Nuevo León | 1.0299 | 1.7441 | 5.8472 | 3,295,727 | 5,091,403 | 5,746,988 |
| Oaxaca | 1.4321 | 1.9155 | 5.6428 | 3,351,116 | 4,468,621 | 5,345,223 |
| Puebla | 1.1844 | 1.8226 | 3.3194 | 3,118,334 | 4,203,434 | 4,716,775 |
| Querétaro | 1.8686 | 1.9423 | 3.1726 | 3,014,141 | 4,044,314 | 4,964,295 |
| Quintana Roo | 1.4429 | 1.7423 | 2.0684 | 3,586,124 | 4,742,665 | 5,294,139 |
| San Luis Potosi | 1.7737 | 2.8752 | 6.2566 | 3,191,184 | 4,227,360 | 5,281,403 |
| Sinaloa | 1.0626 | 1.7840 | 5.3023 | 3,114,738 | 5,218,369 | 6,013,151 |
| Sonora | 1.6363 | 1.7240 | 2.4131 | 3,228,770 | 4,232,978 | 5,663,063 |
| Tabasco | 1.1710 | 1.9294 | 5.2025 | 2,837,561 | 5,661,566 | 5,805,680 |
| Tamaulipas | 1.5596 | 2.1749 | 4.7739 | 2,774,473 | 4,219,399 | 5,412,481 |
| Tlaxcala | 1.1990 | 2.3662 | 3.8524 | 3,637,129 | 3,940,252 | 5,529,762 |
| Veracruz | 1.5245 | 2.4462 | 3.8524 | 3,555,363 | 4,380,884 | 5,529,762 |
| Yucatán | 1.7277 | 1.7537 | 4.0851 | 2,912,581 | 4,758,504 | 5,425,127 |
| Zacatecas | 1.4006 | 2.3769 | 2.0330 | 2,823,526 | 4,109,925 | 6,044,991 |

the obtained product for each of processing routes and processing facilities. Also, Table 2 shows the unit operating cost for each processing route.

It is important mention that the mathematical model does not have embedded thermodynamic constraints because the main goal of the paper is the planning problem that does not need thermodynamic constraints (see Supply Chain Planning Problem subsection into literature review). However, these constraints and parameters are crucial when any processing system is modelled. In particular, the data used were rigorously obtained through the Aspen Plus simulator. To obtain the appropriate conversion factors used in the process units, the simulator rigorously and robustly solves the MESH equations (material, energy, thermodynamic equilibrium, summation constraints). Particularly, regarding the thermodynamic model, the NRTL-HOC model was used. To ensure the reliability of the data, Fig. 2 shows the direct comparison between the experimental data used and the data generated by the Aspen Plus modelling. Fig. 2 illustrates the experimental composition of the binary system n-butanol/water (the system with the interest compounds) [63] acquired at temperatures ranging from 323 to 393 K and pressures ranging from 13.4 to 267 kPa, as well as the data predicted by the NRTL model using default Aspen Plus binary interaction parameters. In addition, prior research has found that predicting the interactions between the components is relatively accurate [64,65]. Even though these parameters could be obtained from literature or experimental information if these are available.

Other important parameters are the product demand and product price for each product type and consumption region. Product demand and product price data are provided in Table 6. As can be seen, the demand is huge and then the demand is not limiting the product production [see Equation (10)]. The production is limited by raw material availability and processing capacity in each processing plant.

Regarding the capital costs, Table 7 presents the lower and upper bounds for processing technologies as well as the fixed and variable capital costs for each technology.

### 6.1. *Case study remarks*

It is worth noting that the case study is hypothetical, and the mathematical model is fed from official data and results from simulations to try to be realistic as much as possible. This is a weakness of any similar approach since the quality of results is strongly dependent on the quality of inputs. Hence, an important assumption for case study data is the product demand because this parameter was estimated from other products with similar use. It is needed to mention that the database applies for the year 2018 because of data availability and then product demand is assumed to be constant since 2018 (see Ref. [66]).

## 7. Results and discussion

The described case study was implemented in the software GAMS and it was formulated as a Mixed Integer-Non-Linear Problem. The model consists of 1967 constraints, 12,590 continuous variables and 384 binary variables. We used a CPU with i7-7500U processor and 8 GB of RAM at 3.2 GHz, which consumed around 0.200 s per point in each Pareto curve using a combination of BARON and DICOPT solvers. The main results are presented along this section.

### 7.1. *Maximization of net profit and environmental impact*

Because of mathematical formulation has three objectives a multi-objective approach should be applied: 1.- Net annual profit (NP), 2.- Net CO2 equivalent emissions (EMISS), and 3.- Social objective function associated to location (SOL). Herein, it could be difficult to observe the behavior of all three objectives when they are maximized via a

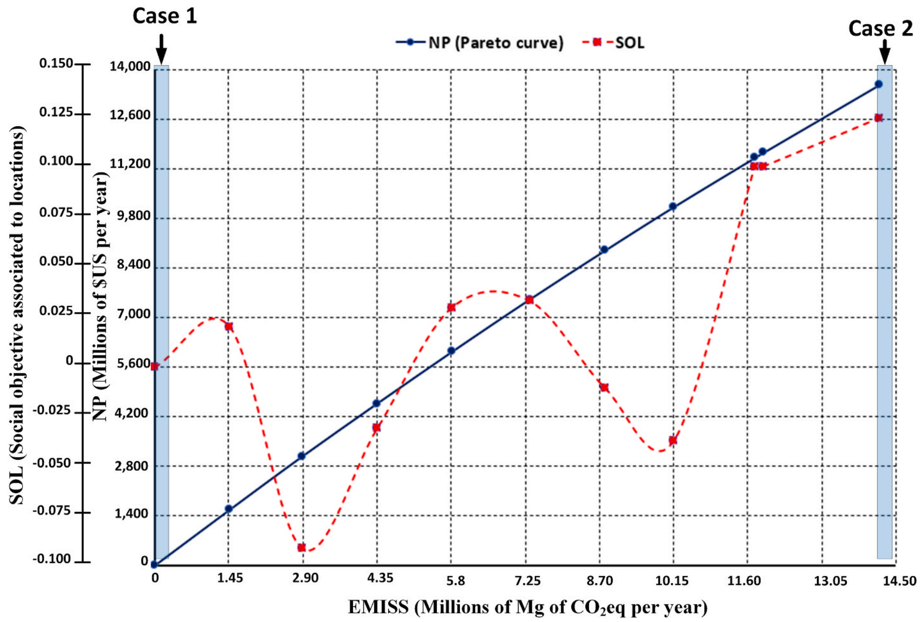


**Fig. 3.** Pareto curve between NP and EMISS. Additional curve corresponds to social objective associated to supply chain locations.

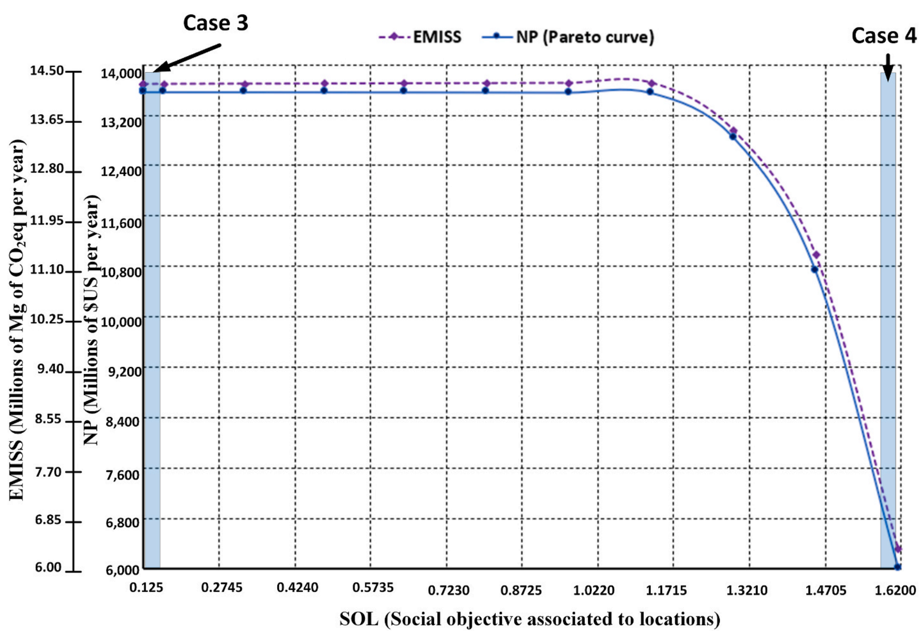


**Fig. 4.** Pareto curve between NP and SOL. Additional curve corresponds to net emissions.

conventional Pareto curve analysis. It is important to mention that different cases for specific solutions are identified in each generated Pareto curve.

For this case study, Fig. 3 shows the behavior of Pareto front between the environmental impact and the net annual profit is almost linear and its correlation is positive, in which the maximum reached value for EMISS is 14.17 Million of $CO_2$ emissions in tons per year, whereas the maximum NP is around $US13,572 Million per year. It should be noticed that behavior for social objective and net profit is not linear.

The maximum achieved value for SOL is around 0.1250 with 19 selected harvesting sites and 32 selected processing plants that corresponds to the maximum net profit point (see Case 2 in Fig. 3). It is important to note that whether the social objective function is zero could means that both terms in social function are equal to zero that occur when all sites are selected. Another possible case corresponds that social terms are nulled each other (social terms could be negative if non marginalized sites are selected). In this case, when social function is equal to zero both terms are nulled each other and then there is not a case where all supply chain sites are selected.

It is worth noting that each point in the Pareto curve represents a different manufacturing system topology, which consists of a different selection of harvesting sites, processing facilities, consumers as well as the amount and type of raw materials and products. For this pairwise analysis, chosen raw material is sugar cane from different selected harvesting but the number of them is different in each Pareto curve region.

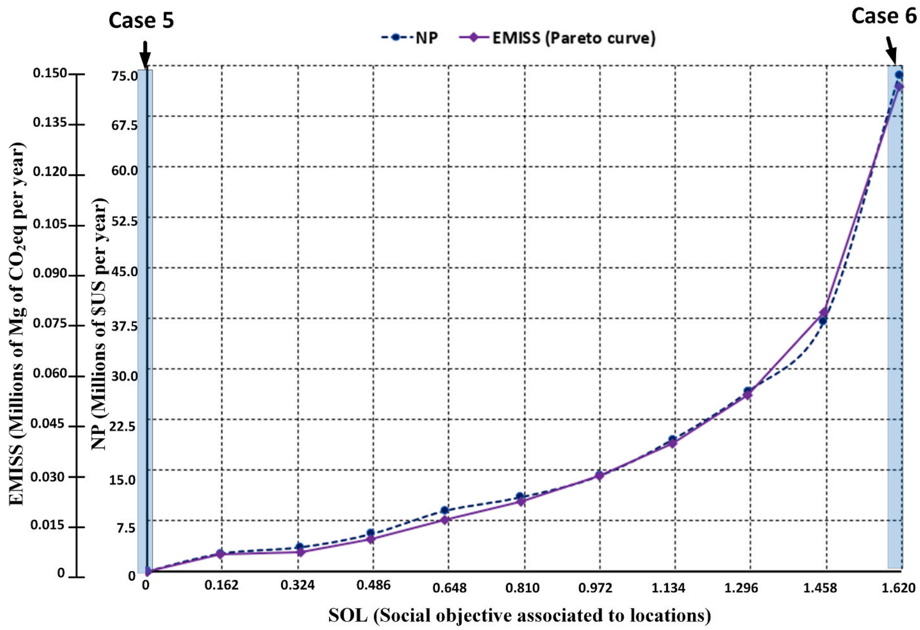


**Fig. 5.** Pareto curve between EMISS and SOL. Additional curve corresponds to net profit.

### *7.2. Maximization of net annual profit and social function for harvesting sites*

Furthermore, Fig. 4 depicts the multi-objective analysis between NP and SOL. It can be seen that it is possible to obtain a value of 13,572 Million of $US per year that is equal to the maximum profit reached in Fig. 3. Also, it is shown that it is possible to obtain a NP close to 6000 Million of $US per year, while the social objective changes significantly from 0.125 up to 1.62. This behavior illustrates that social impact can be significantly increased if the net profit decrease around 55.8% the reason for these variations might be caused by different locations for harvesting sites and processing plants. In this case, the locations with the highest marginalization level are preferred (in Fig. 3 the social function is not optimized).

Concerning EMISS, this objective shows a similar behavior by comparison with NP. . At this point, we can claim that similar values for economic and environmental functions could be obtained with a specific supply chain configuration. However, the social impact can be enhanced whether social aspect is involved in the multi-objective analysis.

### *7.3. Minimization of environmental impact and maximization of social function*

Fig. 5 presents the tradeoff between EMISS and SOL. This multi-objective analysis illustrates that it is possible to obtain a trade-off between social and environmental objectives. The maximum obtained value for SOL (for this multi-objective analysis) was around 1.62 while the maximum value of EMISS is around $1.5 \times 10^5$ Mg per year.. It is worth noting that $1.5 \times 10^5$ Mg per year is negligible compared with 14 $\times$ $10^6$ Mg per year that corresponds to other multi-objective analyses (see Fig. 3).

Additionally, the $CO_2$ emissions and net profit have a similar behavior when a multi-objective analysis between SOL and EMISS is done. This might mean that for that case the economic objective could not be considered as an additional objective in the entire problem.

Finally, it is essential to mention that achieved maximum values for EMISS and NP are approximately $1.5 \times 10^5$ Mg per year and $US 73.6 $\times$ $10^6$ per year respectively, which are insignificant when they are compared with obtained values in previously discussed pairwise analyses.

### *7.4. Selection of a solution based on pairwise analysis*

It is worth noting that points in Pareto curves correspond to optimal solutions when different objectives are analyzed. These points can be global optimal or suboptimal solutions because of the model is MINLP [see Equation (5)], to ensure that only global optimal or suboptimal solutions have been found, the model status was verified and, in case that obtained solution were not at least suboptimal, the solver was changed and used different initial values for variables.

Additionally, when supply chain planning problem is addressed, the aim is to obtain global optimal solutions. However, our model is MINLP

**Table 8**
Summary for the solutions for all multi-objective analyses.

| Pairwise comparison | Case | NP (Millions of $US per year) | EMISS (Millions of Mg per year) | SOL (Social objective associated to locations) | Comments |
|---|---|---|---|---|---|
| NP vs EMISS | Case 1 | 13,572 | 14.17 | 0.13 | Linear behavior between NP and EMISS |
| | Case 2 | 0 | 0 | 0.00 | |
| NP vs SOL | Case 3 | 13,572 | 14.17 | 0.13 | EMISS objective could be omitted because of its behavior. |
| | Case 4 | 6017 | 6.34 | 1.62 | |
| SOLvs EMISS | Case 5 | 0 | 0.00 | 0.00 | Profit objective could be omitted because of its behavior. |
| | Case 6 | 74 | 0.14 | 1.62 | |
| ALL | Max value | 13,572 | 14.18 | 1.62 | Points obtained from all points in all pairwise analyses |
| | Min value | 0 | 0.00 | 0 | |

**Table 9**
Satisfaction level for each multi-objective analysis.

| Case | NP | EMISS | SOL | Average |
|---|---|---|---|---|
| Case 1 | 100.00 | 0.06 | 7.74 | 35.93 |
| Case 2 | 0.00 | 100.00 | 0.00 | 33.33 |
| Case 3 | 100.00 | 0.00 | 7.74 | 35.91 |
| Case 4 | 44.33 | 55.29 | 100.00 | 66.54 |
| Case 7 | 0.00 | 100.00 | 0.00 | 33.33 |
| Case 8 | 0.54 | 98.99 | 100.00 | 66.51 |

and then it sometimes is not possible. For that reason, the strategy considers generation of several Pareto curves to do a more complete scanning of the feasible region.

A disadvantage of generators methods is that these algorithms do not provide a unique solution and an additional analysis should be carried out to be able to suggest a solution to stakeholders. Nevertheless, it is possible to recommend a solution to decision makers if all pairwise analyses are considered. In this respect, Table 8 contains a summary for all values for NP, EMISS and SOL for all pairwise analyses. It can be observed that in cases where SOL is maximized the objectives EMISS or NP have similar behaviors and one of these objectives could be omitted in the multi-objective analysis and therefore, optimization problem could be considered as a problem with two objectives instead of three.

In addition, based on generated Pareto curves, it is possible to obtain the maximum and minimum values for objectives in order to normalize obtained values and to obtain the satisfaction level for each objective in each potential solution. Satisfaction level for each objective is a measure to determine if an objective is near or far from its best-found value. Satisfaction levels for each objective are defined as follows:

$$SatisfactionNP^{solution} = 100\left[\frac{NP^{solution} - NP^{MIN}}{NP^{MAX} - NP^{MIN}}\right] \quad (30)$$

$$SatisfactionEMISS^{solution} = 100\left[\frac{EMISS^{MAX} - EMISS^{solution}}{EMISS^{MAX} - EMISS^{MIN}}\right] \quad (31)$$

$$SatisfactionSOL^{solution} = 100\left[\frac{SOL^{solution} - SOL^{MIN}}{SOL^{MAX} - SOL^{MIN}}\right] \quad (32)$$

Table 9 presents the satisfaction level for each objective and extreme cases in Pareto curves. Also, Table 9 shows the average satisfaction level considered as the arithmetic average of satisfaction level for each objective. It is observed that potential solution with the highest satisfaction level is the case 4 in which the social objective and the net profit are analyzed. satisfaction level for this case is around 66.54%. Fig. 6 illustrates the covered surface for each potential solution based on the satisfaction level in which is observed that maximum covered surface corresponds to the same mentioned case (see Case 4).

As mentioned, each obtained solution from pairwise analyses can be normalized. Based on maximum and minimum values for objectives it can be defined a hypothetical point with 100% of satisfaction for each objective, which is known as utopic point since if there is a tradeoff between objectives it not possible to obtain that solution.

An additional strategy is to obtain the normalized distance of each Pareto point with the utopic point in order to choose a solution. This strategy allows selecting one of the optimal solutions from the multi-objective analyses and therefore to analyze in detail that solution to give a suggestion for stakeholders. This procedure was based on the approach proposed by Ref. [67].

Hence, utopic regards to NP equal to 13,572 Million of $US per year, EMISS equal to zero $CO_2$ emissions, and SOL equal to 1.62. Based on this

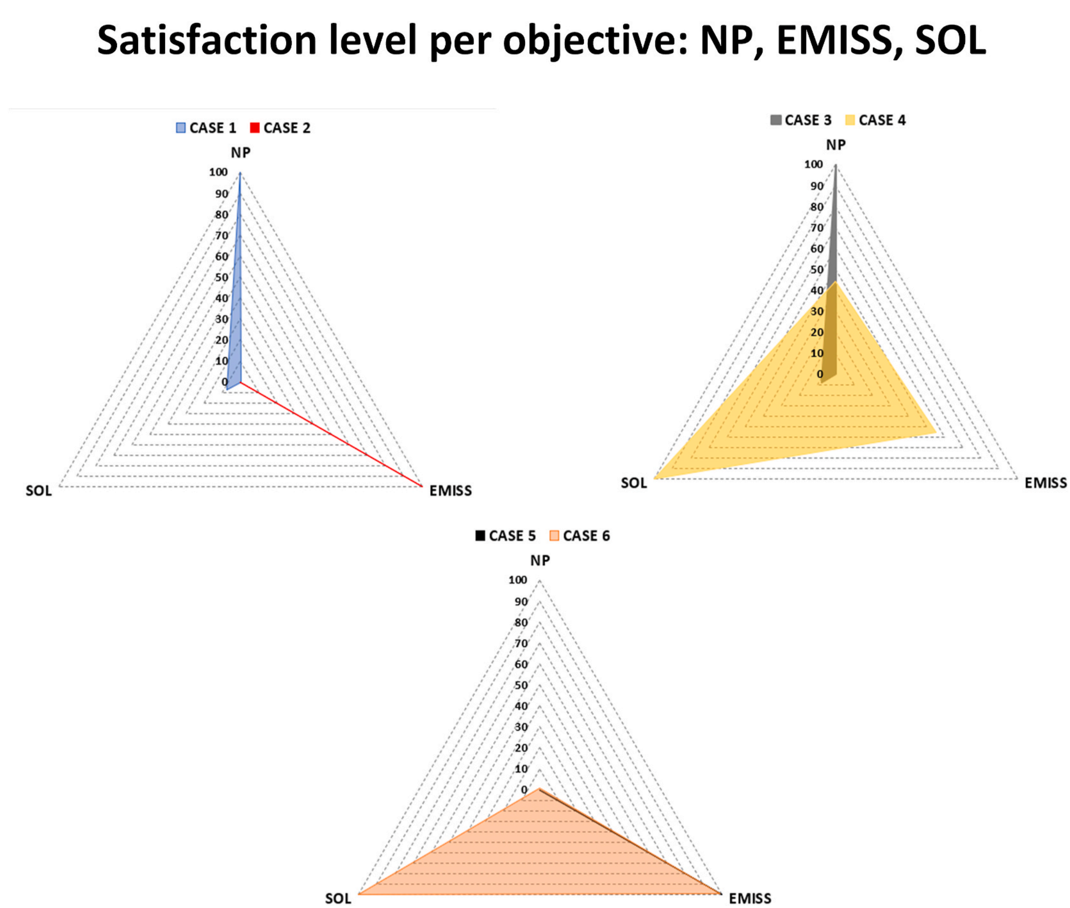


**Fig. 6.** Satisfaction level for each objective as covered surface for cases described in Tables 8 and 9 Solutions were obtained from pairwise analyses.

**Table 10**
Amount of used raw material according the closest solution to the utopic point.

| Raw material | Used amount (Mg/y) | 100*(used amount/ available amount) | Number of sites where is supplied |
|---|---|---|---|
| Wheat straw | 1680 | 0.038 | 14 |
| Sugar cane | 690,760 | 1.22 | 12 |
| Wheat | 1680 | 0.07 | 14 |
| Corn grain | 1680 | 0.01 | 14 |
| Sorghum grain | 840 | 0.02 | 7 |
| Cassava root | 0 | 0.00 | 0 |
| Sugar beet | 1680 | 0.72 | 14 |
| Sweet sorghum | 1680 | 0.27 | 14 |
| Total | 700,000 | 0.77 | 14 |

analysis, the closest point with the utopic point corresponds as follows: NP equal to $US 6017 million per year, EMISS equal to 6.34 million of $CO_2$ Mg per year, and SOL equal to 1.62. In conclusion, all considered ways to choose a solution suggest the same potential solution.

Specifically, the closest point to the utopic point considers 14 harvesting sites and 14 processing facilities. Moreover, this point suggests processing 700,000 Mg per year that corresponds to 7 raw materials. Selected raw material are a) wheat straw, b) sugar cane, c) wheat grain, d) corn grain, e) sorghum grain, f) sugar beet and g) sweet sorghum. Table 10 presents in detail the amount of these raw materials. As can be seen, the amount of used raw material represents 0.77% of total available raw material that might imply a low effect in other competitive raw material uses. The main raw material is the sugarcane with 690,760 Mg/y (1.22% of total available).

Table 11 presents the chosen locations for harvesting sites and the obtained amount of raw material. It is possible to observe that sites with high marginalization level such as Chiapas (MI = 2.41), Michoacán (MI = 0.5), and Oaxaca (MI = 2.12) were selected. Michoacán and Chiapas are the locations with the highest mass amount of raw materials that are mainly composed by sugar cane. It is worth noting that even though Veracruz (MI = 1.14) is the state with highest sugar cane production in Mexico, the sugar cane used by the proposed supply chain is supplied by the Michoacán and Chiapas region because marginalization index for Veracruz is lower than that index for Chiapas. Thus, mathematical approach prioritizes to use raw materials from locations with high marginalization level.

Table 12 shows the used raw material to be processed in processing facilities. Alike the harvesting sites, the processing facilities are locations with high marginalization level. All capacity for processing facilities are equal and the main raw material is the sugar cane.

## 8. Managerial insights

Our mathematical model for de planning for ABE process considering sustainability issues through four objectives is applicable to different raw materials, products and processing routes, therefore it can be applied to other supply chains.

Multiple multi-objective analyses allow generating several local optimal solutions which can be evaluated via a satisfaction factor or distance to utopic point.

Multiple pairwise analyses help to find uncommon relationships between objective functions that in some cases do not exist a predictable behavior.

If social objective is maximized, the obtained solution will promote the selection of marginalized locations for processing plants and harvesting sites and behavior for economic and environmental objective is similar.

By examination of selected solution of our mathematical model, it can be observed that the limiting parameters for addressed supply chain

**Table 11**
Amount of supplied raw material according the closest solution to the utopic point (Mg/y).

| Suppliers | Total Raw Material | Wheat straw | Sugar cane | Wheat grain | Corn grain | Sorghum grain | Sugar beet | Sweet sorghum |
|---|---|---|---|---|---|---|---|---|
| Campeche | 960 | 120 | 240 | 120 | 120 | 120 | 120 | 120 |
| Chiapas | 42,440 | 120 | 41,720 | 120 | 120 | 120 | 120 | 120 |
| Durango | 720 | 120 | 0 | 120 | 120 | 120 | 120 | 120 |
| Guerrero | 2582 | 120 | 1862 | 120 | 120 | 120 | 120 | 120 |
| Hidalgo | 720 | 120 | 0 | 120 | 120 | 120 | 120 | 120 |
| Michoacán | 50,720 | 120 | 50,000 | 120 | 120 | 120 | 120 | 120 |
| Nayarit | 960 | 120 | 240 | 120 | 120 | 120 | 120 | 120 |
| Oaxaca | 720 | 120 | 120 | 120 | 120 | 0 | 120 | 120 |
| Puebla | 720 | 120 | 120 | 120 | 120 | 0 | 120 | 120 |
| San Luis Potosi | 840 | 120 | 240 | 120 | 120 | 0 | 120 | 120 |
| Tabasco | 720 | 120 | 120 | 120 | 120 | 0 | 120 | 120 |
| Veracruz | 720 | 120 | 120 | 120 | 120 | 0 | 120 | 120 |
| Yucatán | 720 | 120 | 120 | 120 | 120 | 0 | 120 | 120 |
| Zacatecas | 720 | 120 | 120 | 120 | 120 | 0 | 120 | 120 |

**Table 12**
Amount of used raw material in processing facilities according the closest solution to the utopic point (Mg/y).

| Region | Total Raw Material | Wheat straw | Sugar cane | Wheat grain | Corn grain | Sorghum grain | Sugar beet | Sweet sorghum |
|---|---|---|---|---|---|---|---|---|
| Campeche | 50,000 | 0 | 50,000 | 0 | 0 | 0 | 0 | 0 |
| Chiapas | 50,000 | 0 | 50,000 | 0 | 0 | 0 | 0 | 0 |
| Durango | 50,000 | 0 | 50,000 | 0 | 0 | 0 | 0 | 0 |
| Guerrero | 50,000 | 1680 | 41,600 | 1680 | 960 | 840 | 1560 | 1680 |
| Hidalgo | 50,000 | 0 | 50,000 | 0 | 0 | 0 | 0 | 0 |
| Michoacán | 50,000 | 0 | 50,000 | 0 | 0 | 0 | 0 | 0 |
| Nayarit | 50,000 | 0 | 50,000 | 0 | 0 | 0 | 0 | 0 |
| Oaxaca | 50,000 | 0 | 50,000 | 0 | 0 | 0 | 0 | 0 |
| Puebla | 50,000 | 0 | 50,000 | 0 | 0 | 0 | 0 | 0 |
| San Luis Potosi | 50,000 | 0 | 49,880 | 0 | 120 | 0 | 0 | 0 |
| Tabasco | 50,000 | 0 | 50,000 | 0 | 0 | 0 | 0 | 0 |
| Veracruz | 50,000 | 0 | 50,000 | 0 | 0 | 0 | 0 | 0 |
| Yucatán | 50,000 | 0 | 49,520 | 0 | 360 | 0 | 120 | 0 |
| Zacatecas | 50,000 | 0 | 49,760 | 0 | 240 | 0 | 0 | 0 |

is not the biomass availability since used biomass regards to maximum 1.22% of available biomass for sugar cane.

## 9. Conclusions

This manuscript has presented a mathematical model for planning a supply chain for production of acetone, butanol and ethanol through multiple biomass feedstocks. The proposed model took into account four objective functions related with sustainability dimensions in order to address some of the United Nations Sustainability Development Goals such as: 1.- End poverty in all its forms everywhere because is focused on selected marginalized sites to install the described supply chain and 2.- Ensure access to affordable. Reliable, sustainable and modern energy for all since the considered supply chain might produce two promising biofuels in the world for the transportation field ([7]).

Regarding the general findings for the supply chain planning, it is essential to mention that the determination of processing facilities, harvesting sites, amount of raw material to be used, amount of product to be produced and potential values for economic, environmental and social impact allow to define strategies to decarbonization of technologies, biomass production and product demand forecast. It should be noticed that one of the main advantages is that mathematical formulation and solution is general, and it can be applied to another case study if required, even to other countries with adequate information.

Concerning limitations of proposed approach, one of the major limitations of this study is that the addressed problem is deterministic instead of stochastic and therefore effects of variations in parameters could be missed. Also, another limitation is that model for processing could be oversimplified and the implementation of a processing system might have important deviations. Finally, results depend on reliability of input data and sometimes the information could not be updated such as reports in Marginalization index, which could be updated each five or ten years in Mexico.

Respect to mathematical formulation, this included two social objective functions to promote the selection of sites with high marginalization level when supply chain topology is defined. Based on the obtained results, we can claim that the proposed social objective functions prioritize marginalized locations instead of locations with high biomass availability into the supply chain planning problem.

Also, a practical implication of results is a planning scheme for biomass production, since based on results, the consume of biomass is estimated to be lower than 1% of available biomass in most of cases, and then biomass consume as well as its production might not be seriously affected because the highest percentage of biomass use corresponds to 1.22% for sugarcane and then other competitive uses would should not be affected.

Concerning future works, the social objectives functions can be easily extended to other types of supply chains or production systems considering the location of social impact that is not considered in other works. In addition, results of this study can be used to more specific case studies for other supply chains by reduction of the scale, since if scale is reduced the estimation of transportation cost, biomass availability and even social marginalization could be improved.

## Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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