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# Multiobjective Model for More Sustainable Fuel Supply Chains. A Case Study of the Sugar Cane Industry in Argentina

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**ABSTRACT:** The objective of this work is to present a quantitative tool to support decision-making in the area of optimal design of supply chains (SC) for the combined production of sugar and ethanol. The problem is formulated as a multiobjective mixed-integer linear program that seeks to optimize simultaneously the economic and environmental performance of the production chain. The advantages of the approach presented are illustrated through its application to a case study, in which a trade-off exists between the economic and environmental performance of the network. Our method provides valuable insight into the problem and a guide to adopt more sustainable strategic alternatives in the design of SCs with embedded biorefineries.

## INTRODUCTION

Bequeathing to future generations a suitable environment for the continuity of civilization has become a major concern. This has led to the concept of sustainability, first introduced in the Brundtland report.<sup>1</sup> Von Blottnitz and Curran<sup>2</sup> emphasized that moving toward “sustainability” requires a rethinking of our systems of production, consumption, and waste management. In the context of economic globalization, it is not possible to stand apart from this general trend. Particularly, there is nowadays an increasing awareness about the future reduction of fossil energy resources, such as those coming from oil. In this scenario, consumers and governments are becoming increasingly concerned about environmental protection issues. The perception that improving the sustainability of a production process could simultaneously improve its economic performance, has also been the driving force for adopting more sustainable production patterns in process industries. For these reasons, renewable fuels have gained wider interest in the recent past, bioethanol being one of the most successful examples of a global shift from fossil sources of energy to biobased fuels.

The use of ethanol in vehicles was first proposed by Henry Ford in 1896. After the oil crisis, ethanol became more popular, since oil-importing countries were forced to develop alternative fuel programs in order to reduce their dependence on oil. Over the last decades, vast investments, government sponsorship, and tax incentives made Brazil and United States the world leaders in ethanol production. As a result, they now hold about 90% of the world's ethanol production.

In Brazil, a sugar cane-based bioethanol policy was implemented four decades ago (National Pró-Álcool Programme, 1975). In this country, a mixture of 25% alcohol is used in the transportation sector, and 80% of the vehicles can operate under the “flex-fuel” mode; that is, they can either use gasoline, ethanol, or a mixture of both.<sup>3</sup> In 1978, USA approved the Energy Tax Act to promote the usage of renewable energy through taxes and tax credits. In 2009, the total annual capacity of bioethanol was 40 125 million liters, most of which were produced in corn-based distilleries.<sup>4</sup>

Many countries have launched programs to replace gasoline by ethanol in the midterm. China, India, Colombia, Thailand, Mexico, and Venezuela<sup>5</sup> are examples of this general trend. Argentina published law 26 093 in 2006, which provides the framework for investment, production, and marketing of biofuels. This law, which became active in 2010, establishes a minimum content of biofuel in gasoline and diesel (i.e., 5%). The main goal is to diversify the supply of energy and to promote the development of rural areas, especially in benefit of small- and medium-sized agricultural producers. Most of the ethanol in Argentina is currently produced by 15 sugar mills located in the northwest of the country that use sugar molasses as main feedstock. To meet the official requirements, Argentina needs to expand its sugar cane industry in order to produce approximately 270 million liters of ethanol per year for blending.

Argentina has abundant natural resources, a very efficient agricultural production sector, and good processing and export infrastructures.<sup>6</sup> The sugar cane industry is becoming aware of the role that this grass will play in the future, given its resistance, rapid growth, and uptake capacity for atmospheric carbon. The ethanol production from sugar cane has a virtually positive energy balance, which can help to mitigate global warming. Furthermore, ethanol also leads to less CO, SO<sub>x</sub> and VOC emissions when it is used in combustion engines. Ethanol has also better antiknock characteristics than gasoline, and its higher autoignition temperature and flash point make it safer than gasoline.<sup>7</sup>

Nevertheless, there are some drawbacks associated with this biofuel, such as the land competition with food, the environmental impact associated with the transport sector, and the

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generation of large amounts of wastewater during the production process. In addition to this, the rapid expansion of ethanol production/consumption has affected the international market of sugar, a coproduct of ethanol in the Argentinean sugar cane industry. Such a complex environment poses significant challenges for practitioners and researchers. In particular, one of the key issues that still remains open is how to develop a more comprehensive approach to design infrastructures capable of meeting the growing demand of sugar and ethanol in a sustainable manner. This design task is further complicated by the need to account for different conflictive criteria at the early stages of the process development.

Decisions involved in the design, planning, production, and delivery of products to final customers are the focus of supply chain management (SCM). In the last few decades, the process systems engineering community (PSE) has developed tools to facilitate decision-making in this area. This paper focuses on the use of mathematical programming for optimizing strategic and tactical decisions in the sugar cane industry. Decisions at these levels have a long lasting effect on the firm, and hence play an extremely important role in SCM.

As mentioned before, environmental aspects should be considered along with the economic performance when designing energy systems. The need to account for environmental concerns in SCM has led to the concept of green supply chain management (GrSCM). The PSE literature on GrSCM is quite scarce. Nevertheless, it is expected that this area will be the focus of intensive research in the near future.<sup>8</sup> An extensive review with more than 200 citations related to GrSCM can be found in the work by Srivastava.<sup>9</sup> The author points out that mathematical programming has not been extensively used in the design of environmentally conscious SCs.

Few works have focused on the optimization of bioethanol/sugar SCs. Particularly, Yoshizaki et al.<sup>10</sup> introduced a linear programming (LP) model to find the optimal distribution of sugar cane mills, fuel bases and consumer sites in southeastern Brazil. Kawamura et al.<sup>11</sup> presented an LP model to minimize the transportation and storage costs of the existing sugar cane SC in Brazil. Ioannou<sup>12</sup> applied an LP model to reduce the transportation costs in the sugar beet industry in Greece. The mixed-integer linear programming (MILP) model proposed by López Milán et al.<sup>13</sup> minimizes the transportation cost of the sugar cane SC in Cuba. Dunnett<sup>14</sup> et al. developed a model to find the optimal configuration of a lignocellulosic bioethanol network. Zamboni et al.<sup>15</sup> presented an MILP model to minimize the cost of a static corn-based bioethanol SC. Mathematical programming methods associated with plantation planning and scheduling can also be found in the works by Grunow et al.,<sup>16</sup> Paiva and Morabito,<sup>17</sup> Colin,<sup>18</sup> and Higgins and Laredo.<sup>19</sup> As observed, most of these contributions have mainly focused on studying the individual components of the ethanol SC rather than on optimizing all its single entities in an integrated manner.

One of the approaches that has gained wider interest in GrSCM in the recent past is the combined use of mathematical programming and life cycle assessment,<sup>20</sup> a framework that was formally introduced by Azapagic and Clift.<sup>21</sup> This integrated framework allows an automation of the search for alternatives leading to life cycle environmental savings. The works by Hugo and Pistikopoulos,<sup>22</sup> Bojarski et al.,<sup>23</sup> and Guillén-Gosálbez et al.<sup>24</sup> are examples of the application of this general approach to process industries. Very few works have addressed the multi-objective optimization of bioethanol SCs with economic and

LCA-based criteria. Buddadee et al.<sup>25</sup> proposed a multiobjective optimization model for the sugar cane industry in Thailand, considering two options for the excess of bagasse: electricity generation or ethanol. The model was based on an existing network of sugar mills that was analyzed under steady state conditions. An economic indicator and the global warming potential assessed from a life cycle perspective were the objectives to be optimized. Zamboni et al.<sup>26</sup> presented a multiobjective framework to optimize the design of the corn-based ethanol SC in northern Italy, as an extension of a former article.<sup>15</sup> They also considered economic and environmental metrics in the optimization.

In contrast to these approaches, the works by Beeharry,<sup>27</sup> Ramjeawon,<sup>28</sup> Botha and von Blottnitz,<sup>29</sup> and Renouf et al.<sup>30</sup> focused on assessing the life cycle impact of ethanol production from sugar cane. In the same line, Contreras et al.<sup>31</sup> applied LCA to decide among different alternatives of sugar cane processing. This work focused at the single plant level, neglecting the impact caused in other echelons of the production chain. To the best of our knowledge, there is no study that integrates multiobjective optimization and LCA for the analysis of sugar cane SCs.

The aim of this work is to develop a quantitative decision-support tool based on mathematical programming for the design of more sustainable SCs belonging to the sugar cane industry. Our approach relies on an holistic formulation that integrates all the components of the sugar cane SC into a single framework. The design task is posed in mathematical terms as a bicriteria mixed-integer linear programming problem (bi-MILP) that seeks to maximize the net present value of the SC and minimize its environmental impact. The latter criterion is measured in this work according to LCA principles. The capabilities of the proposed approach are illustrated through a case study based on the Argentinean sugar cane industry, for which valuable insight is obtained.

The remainder of this article is organized as follows. The problem statement and modeling assumptions are briefly described. The focus then turns to the application of LCA to our problem, and the proposed mathematical model is presented. This model is then illustrated through a case study based on the Argentinean sugar cane industry. The conclusions of the work are finally drawn in the last section of the paper.

## ■ PROBLEM STATEMENT

In our analysis, we consider, without loss of generality, a generic three-echelon SC (production–storage–market) like the one depicted in Figure 1. This network includes a set of sugar cane producers, production, and storage facilities, and final markets. We assume that we are given a time horizon divided into a set of time periods, and a specific geographic area divided into a set of regions where the facilities of the SC can be established. We consider that each region has an associated sugar cane crop capacity in every time interval. Sugar cane can be either converted into sugar or ethanol. The byproduct from sugar production, mainly molasses and honey, can also be fermented to produce bioethanol. A number of emissions and wastes are generated during the production tasks. Final products (ethanol and sugars) are stored in warehouses before being delivered to the final markets. The SC facilities are connected through transportation links. We consider three types of vehicles: heavy open-box trucks for sugar cane, medium-sized trucks for sugars, and tank trucks for ethanol.

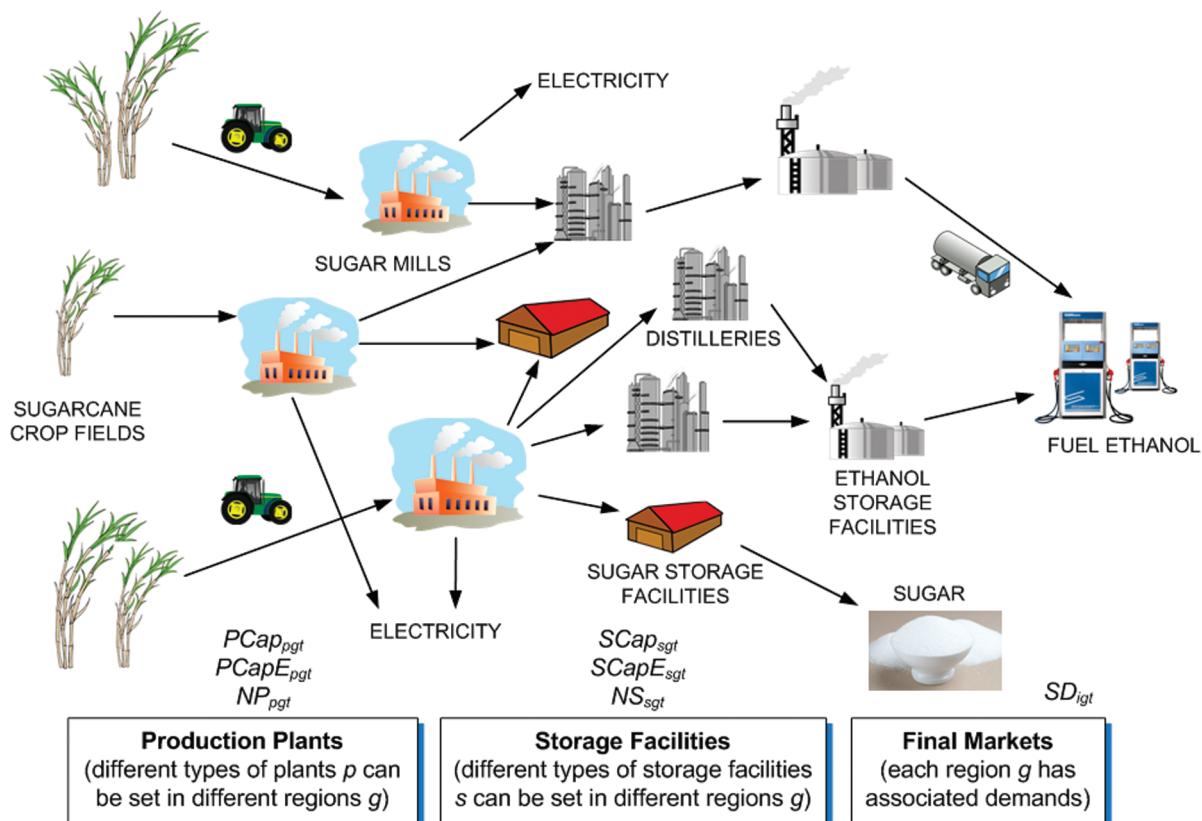


Figure 1. Structure of the bioethanol/sugar SC.

The environmental conscious SC design problem can then be formally stated as follows:

Given are a fixed time horizon, product prices, cost parameters for production, storage and transportation of materials, demand forecast for products, tax rate, capacity data for plants, storages and transportation links, fixed capital investment, interest rate, storage holding period, landfill tax, upper limit on the capital investment, and environmental data (emissions associated with the network operation and damage assessment model).

The goal of the study is to determine the configuration of the three-echelon bioethanol network and associated planning decisions that maximize the net present value and minimize the environmental impact. Decisions to be made include the number, location, and capacity of the production plants, and warehouses to be set up in each region, their capacity expansion policy for a given forecast of prices and demand over the planning horizon, the transportation links and transportation modes that need to be established in the network, and the production rates and flows of feedstocks, wastes, and final products.

## ■ ENVIRONMENTAL IMPACT ASSESSMENT: APPLICATION OF LCA PRINCIPLES

Since the emphasis in this work is placed on the environmental performance of sugar cane SCs, we will first describe the application of LCA to our process before presenting our multiobjective mathematical formulation. Particularly, the environmental performance of the network is quantified according to some LCA-based metrics, in a similar way as was done before by the authors.<sup>24,32</sup> Here, we integrate our LCA analysis with multiobjective optimization,

following the approach introduced by Azapagic and Clift.<sup>21</sup> Examples on the application of this general framework to other cases can be found elsewhere.<sup>8,22,24,33–36</sup>

More precisely, we optimize the environmental performance of our system according to the following metrics: (1) global warming potential evaluated through the CML methodology and (2) Eco-indicator 99. The CML 2001 methodology includes a set of midpoint impact categories and characterization factors proposed by the CML (Center of Environmental Science of Leiden University).<sup>37</sup> Among these categories, we will focus on climate change, which is determined from the emissions of greenhouse gases to air. We calculate the global warming potential for a time horizon of 100 years (GWP100), expressed in kilograms of carbon dioxide per kilogram of emission (considering a global scale). The Eco-indicator 99 metric (EI99) includes 11 impact categories, which are further aggregated into a single metric.<sup>38</sup>

To calculate these metrics, we follow the first three LCA phases: goal and scope definition, inventory analysis, and impact assessment. The remaining phase, LCA interpretation, is performed in our case by coupling LCA with mathematical programming.

**Goal and Scope Definition.** In this phase, we define the main features of the LCA analysis, mainly the goal of the study, system boundaries, allocation methods, and impact categories, among others. In our specific case, the analysis is restricted to the domain of the sugar cane network. Thus, we perform a “cradle-to-gate” analysis that embraces all the activities of the network, starting from the extraction of raw materials (agricultural stage) and ending with the delivery of the products, sugar and ethanol, to customers.

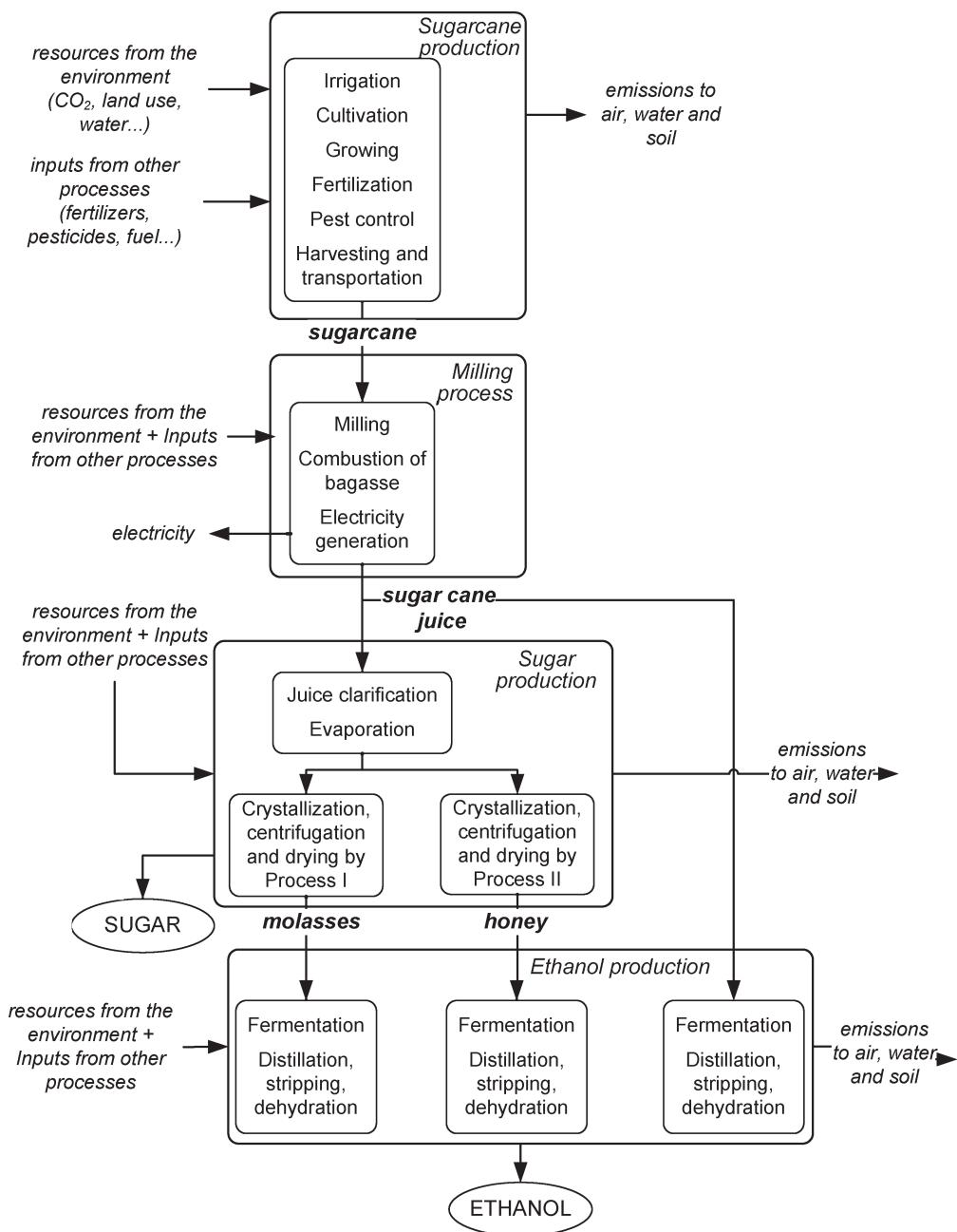


Figure 2. System boundaries considered in the LCA study.

The system under study is the Argentinean sugar cane industry. The overall system has been divided into three subsystems (see Figure 2): (1) Agriculture + Milling, (2) Sugar Production, and (3) Ethanol Production. Tables 1–4 display the main inventory data associated with each subsystem. Note that the boundaries of the analysis have been expanded in order to account for the impact associated with the production of raw materials (e.g., fertilizers, lime, sulfuric acid, etc.). In line with common LCA practice, we have neglected the impact associated with the production of capital equipment. The allocation of byproduct has been avoided whenever possible by expanding the system boundaries. Hence, the environmental load of the byproduct is subtracted from the total environmental load of the process.

The subsystem Agriculture + Milling involves all the activities related to sugar cane planting, growing and harvesting, as well as transportation to sugar mills, sugar cane milling to extract sugar cane juice, and burning of the cellulosic residue, bagasse, in boilers to generate steam and electricity. The electricity production satisfies the sugar mill requirements. The excess of energy is exported to the public network. The conventional sugar cane production in Argentina is characterized by the use of synthetic fertilizers, pesticides, no artificial irrigation, and semimechanized cultivation and harvesting. The ashes from bagasse combustion and filter cake from juice clarification are disposed in the soil replacing some of the synthetic fertilizers used, such as urea and triple super phosphate. Sugar cane is regarded as the main product of the Agricultural stages, whereas sugar cane juice is

**Table 1.** Summary of the Inventory Data for Subsystem Agriculture

	quantity	unit
Inputs		
from the ecosphere		
land use	0.0149	ha·yr <sup>45</sup>
CO <sub>2</sub>	0.8195	t <sup>a</sup>
O <sub>2</sub>	0.1631	t <sup>a</sup>
fueloil	1.7807	t <sup>39</sup>
from the technosphere		
urea	2.9851	kg <sup>b</sup>
superphosphate	0.3582	kg <sup>b</sup>
pesticides	0.2687	kg <sup>b</sup>
filter muds	0.04	t <sup>b</sup>
Outputs		
emissions to the water		
pesticides	0.0009	kg <sup>30</sup>
PO <sub>4</sub> <sup>3-</sup>	0.3821	kg <sup>30</sup>
NO <sub>3</sub> <sup>-</sup>	0.194	kg <sup>30</sup>
emissions to the air		
O <sub>2</sub>	0.596	t <sup>a</sup>
CO <sub>2</sub>	192.5513	kg <sup>a</sup>
CO	21.7362	kg <sup>a</sup>
NO <sub>x</sub>	1.024	kg <sup>30</sup>
SO <sub>x</sub>	0.062	kg <sup>39</sup>
N <sub>2</sub> O	0.2	kg <sup>30</sup>
NH <sub>3</sub>	0.0776	kg <sup>30</sup>
particles	15.004	kg <sup>b</sup>
emissions to the soil		
ash	5.673	kg <sup>b</sup>
harvest trash	155	kg <sup>b</sup>
products		
sugar cane	1	t

<sup>a</sup> Carbon balance calculations (photosynthesis + respiration + combustion). <sup>b</sup> Technical Reports of the Sugar Cane Industry; University Nacional de Tucumán, 2010.

the main product in the Milling stages. In this subsystem, generated electricity has been regarded as a subproduct whose allocation has been solved by expanding the system boundaries, and retrieving the necessary data from the Ecoinvent Database.<sup>39</sup>

The subsystem Sugar Production considers the purification and concentration of sugar cane juice to obtain dry crystals of sugar. There is only one process to carry out the purification (sulfitation, liming, heating, sedimentation and filtering). On the other hand, there are two ways to concentrate the clarified juice to produce sugar. The first technology yields sugar and molasses, while the second one produces sugar and a secondary honey. White sugar has been taken as the main product of this subsystem. Allocation between white and raw sugar has been done in a mass basis.

In the subsystem Ethanol Production, we can use three different technologies depending on the raw material arriving to the distillery: molasses, secondary honey, or sugar cane juice. All of these technologies consume the same inputs (e.g., water, yeasts, etc.), but the consumption rates differ in each case. These technologies lead in turn to different emissions (i.e., CO<sub>2</sub>, VOCs, fusel oil, etc.). The most harmful residue is the vinasses, the properties of which depend on the raw material used in the process. Currently, each ethanol company in Argentina implements a different waste disposal option. In this study, we have considered an average impact for disposing vinasses in soil and surface watercourses.

**Table 2.** Summary of the Inventory Data for Subsystem Milling

	quantity	unit
Inputs		
from the ecosphere		
water	0.4078	t <sup>a</sup>
O <sub>2</sub>	0.0998	t <sup>a</sup>
from the technosphere		
harvested sugar cane	1	t
Outputs		
emissions to the water		
solids	0.0019	t <sup>46</sup>
emissions to the air		
CO <sub>2</sub>	0.2580	t <sup>a</sup>
NO <sub>x</sub>	0.0002	t <sup>46</sup>
SO <sub>x</sub>	0.0001	t <sup>46</sup>
particles	0.0002	t <sup>46</sup>
emissions to the soil		
boiler ash	0.0366	t <sup>b</sup>
products		
electricity to the process	54	MJ <sup>b</sup>
electricity for export	132.12	MJ <sup>b</sup>
LP steam to the process	0.5040	t <sup>b</sup>
sugar cane juice	0.8976	t <sup>b</sup>
bagasse excess	0.02	t <sup>b</sup>

<sup>a</sup> Carbon balance calculations (combustion). <sup>b</sup> Technical Reports of the Sugar Cane Industry; University Nacional de Tucumán, 2010.

**Table 3.** Summary of the Inventory Data for Sugar Production

subsystem process I (to molasses)		subsystem process II (to honey)			
quantity	unit	quantity	unit		
Inputs					
steam	3.6425	t <sup>a</sup>	steam	3.7290	t <sup>a</sup>
lime	16.6667	kg <sup>a</sup>	lime	20	kg <sup>a</sup>
sulfur	2.5	kg <sup>a</sup>	sulfur	3	kg <sup>a</sup>
O <sub>2</sub>	4.5	kg <sup>a</sup>	O <sub>2</sub>	5.4	kg <sup>a</sup>
flocculant	0.001	kg <sup>30</sup>	flocculant	0.0012	kg <sup>30</sup>
NaOH	0.0014	t <sup>a</sup>	NaOH	0.0016	t <sup>a</sup>
HCl	0.0027	t <sup>a</sup>	HCl	0.0032	t <sup>a</sup>
Outputs					
emissions to the water		emissions to the water			
BOD <sub>S</sub>	0.0021	kg <sup>30</sup>	BOD <sub>S</sub>	0.0026	kg <sup>30</sup>
suspended solids	0.0032	kg <sup>30</sup>	suspended solids	0.0039	kg <sup>30</sup>
inorganic solubles	0.0696	t <sup>39</sup>	inorganic solubles	0.0835	t <sup>39</sup>
emissions to the air			emissions to the air		
SO <sub>x</sub>	0.5	kg <sup>39</sup>	SO <sub>x</sub>	0.6	kg <sup>39</sup>
products			products		
white sugar	1	t	white sugar	1	t
raw sugar	0.176	t <sup>a</sup>	raw sugar	0.18	t <sup>a</sup>
molasses	0.4167	t <sup>a</sup>	honey	0.75	t <sup>a</sup>
filter muds	0.3333	t <sup>47</sup>	filter muds	0.4	t <sup>47</sup>

<sup>a</sup> Technical Reports of the Sugar Cane Industry; University Nacional de Tucumán, 2010.

The functional unit defined for the calculations is the amount of sugar and ethanol produced and delivered to customers during the entire time horizon. Note that the model can decide to leave part of the demand unsatisfied due to limited production capacity or low profitability of the final products. Hence, as oppose to standard LCA studies, in our case the functional unit of the

Table 4. Summary of the Inventory Data for Ethanol Production<sup>a</sup>

subsystem distillery I (from molasses)			subsystem distillery II (from honey)			subsystem distillery III (from sugar cane)		
	quantity	unit		quantity	unit		quantity	unit
Inputs								
steam	5.62	t	steam	5.62	t	steam	5.62	t
molasses	4	t	honey	3.35	t	sugar cane	17.12	t
urea	0.0048	t	urea	0.0048	t	urea	0.0048	t
H <sub>3</sub> PO <sub>4</sub>	0.0004	t	H <sub>3</sub> PO <sub>4</sub>	0.0004	t	H <sub>3</sub> PO <sub>4</sub>	0.0004	t
water	1.84	t	water	1.84	t	water	1.84	t
H <sub>2</sub> SO <sub>4</sub>	0.013	t	H <sub>2</sub> SO <sub>4</sub>	0.013	t	H <sub>2</sub> SO <sub>4</sub>	0.013	t
Outputs								
emissions to the water			emissions to the water			emissions to the water		
vinasse I	14.1304	t	vinasse II	14.1300	t	vinasse III	12.8458	t <sup>48</sup>
pH	4.9		pH	4.8		pH	4.6	
DQO	1.4516	t	DQO	1.4515	t	DQO	1.4516	t
DBO <sub>5</sub>	0.5267	t	DBO <sub>5</sub>	0.5267	t	DBO <sub>5</sub>	0.5267	t
total solids	1.5826	t	total solids	1.5826	t	total solids	0.2216	t
inorganic solids	0.5652	t	inorganic solids	0.5652	t	inorganic solids	0.4352	t
Brix	1.3848	t	Brix	1.3847	t	Brix	0.1939	t
Ca	0.0297	t	Ca	0.0297	t	Ca	0.0169	t
Mg	0.0064	t	Mg	0.0064	t	Mg	0.0032	t
Na	0.0078	t	Na	0.0078	t	Na	0.0027	t
K	0.1950	t	K	0.1950	t	K	0.0682	t
N	0.0219	t	N	0.0219	t	N	0.0055	t
P	0.0016	t	P	0.0016	t	P	0.0011	t
emissions to the air			emissions to the air			emissions to the air		
CO <sub>2</sub>	3.37	t	CO <sub>2</sub>	3.37	t	CO <sub>2</sub>	3.37	t
products			products			products		
ethanol	1	t	ethanol	1	t	ethanol	1	t
ethanol MG	0.1250	t	ethanol MG	0.1250	t	ethanol MG	0.1250	t
fusel oil	0.0017	t	fusel oil	0.0017	t	fusel oil	0.0017	t

<sup>a</sup> Technical Reports of the Sugar Cane Industry; University Nacional de Tucumán, 2010.

problem is not fixed. This provides the model with more flexibility, as it allows us to achieve further reductions in the environmental impact by decreasing the production rates. Nevertheless, the model can be easily modified in order to consider a fixed functional unit. To accomplish this, it suffices to define the demand satisfaction constraint as an equality constraint instead of an inequality equation. Hence, the production rates vary according to the SC structure chosen by the model during the optimization, which seeks to minimize the environmental impact and maximize the economic profit simultaneously.

**Inventory Analysis.** In the second LCA phase, we perform mass and energy balances in order to determine the most relevant inputs and outputs of materials and energy associated with the process (i.e., the life cycle inventory of emissions, waste generated, and feedstock requirements). This information is further translated into a set of environmental impacts in phase three.

The inventory data for our problem were obtained from different sources. With regard to the agricultural stage, we collected data from local agricultural companies and governmental organizations. For the industrial stages, we considered standard mass and energy balance coefficients taken from typical sugar mills and distilleries. Data gaps have been covered using specialized literature, handbooks, and databases, as shown in the inventory tables. For transportation, we have used data from the EcoInvent Database v. 2.0.<sup>39</sup> With regard to data quality, which is a very important issue when performing an LCA study, it varies with the source of information. A detailed description of the data quality, including the treatment of uncertainties, is out of the

scope of this article. Nevertheless, this issue does not affect the development of the methodology here presented.

**Impact Assessment.** In this stage, we determine the environmental impact of the process according to a given damage assessment model. As previously mentioned, here we focus on two LCA metrics: GWP100 and EI99. The damage is determined from the life cycle inventory, by multiplying each life cycle inventory entry with the corresponding damage factor.

The environmental impact calculations were implemented in SimaPro 6.0 LCA software.<sup>40</sup> Particularly, we use (1) the CML 2001 (all impact categories) version 2.04 methodology for calculating the GWP100 metric, and (2) the hierarchist perspective of Eco-indicator 99 methodology with average weighting (H/A) for Human Health, Ecosystem Quality and Resources, for determining the EI99 metric.

**Interpretation.** Finally, in the fourth phase, the results of the LCA analysis are analyzed and a set of conclusions and recommendations for the system are formulated. In this regard, the final goal of LCA is to provide criteria and quantitative measures for comparing different process operation and design alternatives. One of the main shortcomings of LCA is that it lacks a systematic way of generating such alternatives and identifying the best ones. To circumvent these limitations, in this paper we follow a combined approach that consists of integrating LCA and optimization tools within a single decision-making framework, such as former studies have done.<sup>21,22,24,26</sup> Thus, in our work the preferences are articulated in the postoptimal analysis of the Pareto optimal solutions. This approach provides further insights

into the design problem, allowing for a better understanding of the inherent trade-off between economic and environmental criteria.

## MATHEMATICAL MODEL

In this section, we present an MILP formulation that embeds the LCA principles described above. Our MILP is based on the models introduced by Almansoori and Shah,<sup>41</sup> and Guillén-Gosálbez et al.,<sup>24</sup> which address the design of hydrogen SCs. Mass balances are handled following the SC formulation developed by Guillén-Gosálbez and Grossmann for the case of petrochemical SCs.<sup>8</sup>

The model accounts for the option of opening more than one facility in a given region and time period. The environmental concerns are included along with the traditional economic objective, giving rise to a bicriteria decision-making problem. The mathematical formulation considers all possible configurations of the future ethanol/sugar SC as well as all technological aspects associated with the SC performance. The following SC activities found in the Argentinean sugar cane industry are included in the analysis:

**Production.** Sugar cane enters the milling process to obtain juice and a lignocellulosic residue called bagasse. Sugar cane juice is treated afterward in different ways. One option is to use this juice to produce white sugar and raw sugar. There are two technologies realizing this “sugar cane-to-sugar” pathway: one of them generates molasses (T1) as a byproduct, whereas the other one generates a secondary honey (T2). These two byproducts differ in their sucrose content. Molasses is a viscous dark honey whose low sucrose content cannot be recovered by crystallization, while secondary honey is a liquid with a bigger amount of sucrose that leaves the sugar mill before being exhausted by crystallization. As previously mentioned, anhydrous ethanol can be produced by fermentation and following dehydration of molasses (T3), honey (T4) and sugar cane juice (T5). According to this, the model considers five different technologies, two for sugar production and three for ethanol production. Figure 3 shows a representation of each technology, including the mass balance coefficients of the products involved. Bagasse is utilized in the sugar mills for energy generation, so the model includes a set of nine materials: sugar cane, ethanol, molasses, honey, white sugar, raw sugar, vinasse type 1, vinasse type 2, and vinasse type 3. Each plant type incurs fixed capital and operating costs and may be expanded in capacity over time in order to follow a specific demand pattern. The establishment of a plant type is determined from the demand of each region, the ability that the region has to fulfill its internal needs, and the transportation costs.

**Storage.** The model includes two different types of storage facilities: warehouses for liquid products and warehouses for solid materials. For each storage facility type, we define fixed capital and unit storage costs, and lower and upper limits on its capacity expansions. The storage capacity might be expanded in order to follow changes in the demand as well as in the supply.

**Transportation.** Transportation units deliver the final products to customers, supply the production plants with raw materials and dispose the process wastes. The model assumes that the transportation tasks can be performed by three types of trucks: heavy open-box trucks for sugar cane, medium-sized trucks for sugar, and tank trucks for liquid products. Each type of transportation mode has fixed capital and unit transportation costs and lower and upper capacity limits.

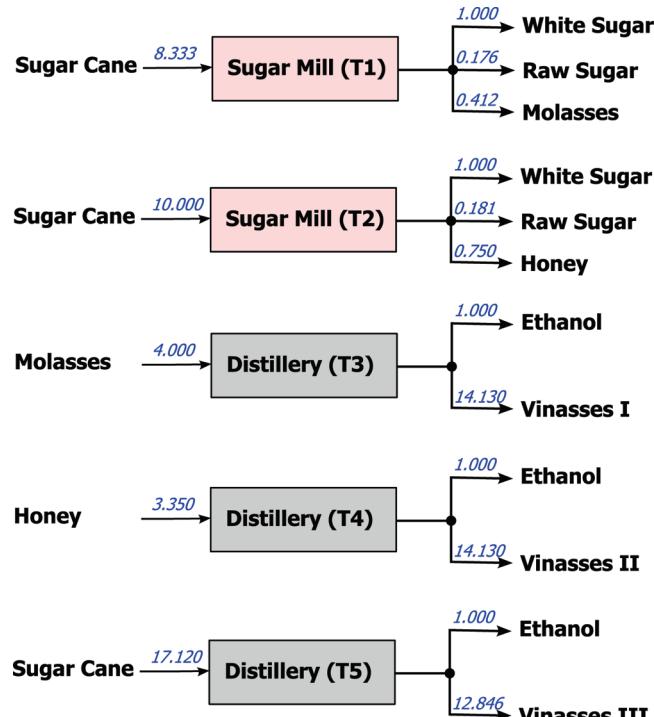


Figure 3. Schematic representation of the five production technologies considered in the SC model with corresponding mass coefficients.

The model includes three main blocks of equations: mass balances constraints, capacity constraints, and objective function equations. An outline of each of these sets of equations is given next.

**Mass Balances Constraints.** The overall mass balance for each region is represented by eq 1. In accordance with it, for every material form  $i$ , the initial inventory kept in region  $g$  from the previous period ( $ST_{isgt-1}$ ) plus the amount produced ( $PT_{igt}$ ), the amount of raw materials purchased ( $PU_{igt}$ ) and the input flow rate from other facilities in the SC ( $Q_{ilgg't}$ ), must equal the final inventory ( $ST_{isgt}$ ), plus the amount delivered to customers ( $DTS_{igt}$ ), plus the output flow to other facilities in the SC ( $Q_{ilgg't}$ ), and the amount of waste generated ( $W_{igt}$ ).

$$\sum_{s \in IS(i,s)} ST_{isgt-1} + PT_{igt} + PU_{igt} + \sum_{l \in IL(i,l)} \sum_{g' \neq g} Q_{ilgg't} = \sum_{s \in IS(i,s)} ST_{isgt} + DTS_{igt} + \sum_{l \in IL(i,l)} \sum_{g' \neq g} Q_{ilgg't} + W_{igt} \quad \forall i, g, t \quad (1)$$

In this equation,  $IS(i,s)$  is a set of ordered pairs that link product  $i$  to the set of suitable storage technologies  $s$ , whereas  $IL(i,l)$  links product  $i$  to its corresponding transportation mode  $l$ . The total production rate of material  $i$  in region  $g$  is determined from the production rates ( $PE_{ipgt}$ ) of each technology  $p$  installed in the region:

$$PT_{igt} = \sum_p PE_{ipgt} \quad \forall i, g, t \quad (2)$$

Note that in Figure 3, the material balance coefficients of the main products (white sugar and ethanol) are normalized to 1. The production rates associated with each technology are

determined from the material balance coefficients,  $\rho_{pi}$ , and the production rate of the main products:

$$\text{PE}_{ipgt} = \rho_{pi} \text{PE}_{i'pgt} \quad \forall i, p, g, t \quad \forall i' \in IM(i, p) \quad (3)$$

In this equation,  $IM(i, p)$  links the main products  $i$  to the corresponding technology  $p$ . The purchases of sugar cane in region  $g$  and time interval  $t$  are limited by the capacity of the existing sugar cane plantation:

$$\text{PU}_{igt} \leq \text{CapCrop}_{gt} \quad i = \text{sugarcane}, \quad \forall g, t \quad (4)$$

The total inventory ( $ST_{isgt}$ ) of product  $i$  stored during time interval  $t$  is limited by the storage capacity ( $SCap_{sgt}$ ):

$$\sum_{i \in IS(i, s)} ST_{isgt} \leq SCap_{sgt} \quad \forall s, g, t \quad (5)$$

During steady-state operation, the average inventory ( $AIL_{igt}$ ) is a function of the amount of material delivered to the customers and the storage period  $\sigma$ :

$$AIL_{igt} = \sigma DTS_{igt} \quad \forall i, g, t \quad (6)$$

Let us clarify that the storage period accounts for the average amount of days that a product will be stored in a given storage facility or warehouse. It is indeed similar to the turnover ratio of a warehouse, which represents the number of times that the stock is completely replaced per time period. To cope with fluctuations in both supply and demand, we assume that the total storage capacity in a region must be at least twice the average inventory level of products  $i$ . Note that here we follow the work by Simchi-Levi et al.<sup>42</sup>

$$2AIL_{igt} \leq \sum_{s \in IS(i, s)} SCap_{sgt} \quad \forall i, g, t \quad (7)$$

Furthermore, the amount of products delivered to the final markets should be less than or equal to the demand ( $SD_{igt}$ ):

$$DTS_{igt} \leq SD_{igt} \quad \forall i, g, t \quad (8)$$

The existence of a transportation link between two regions  $g$  and  $g'$  is represented by a binary variable  $X_{lg'gt}$  which equals 1 if a transportation link is established between the two regions and 0 otherwise. A region can either import or export material  $i$ , but not both at the same time:

$$X_{lg'gt} + X_{lg'gt} = 1 \quad \forall l, t, g, g' (g' \neq g) \quad (9)$$

**Capacity Constraints.** The production rate of each technology  $p$  in region  $g$  is limited by the minimum desired percentage of the available technology that must be utilized,  $\tau$ , multiplied by the existing capacity (represented by the continuous variable  $\text{PCap}_{pgt}$ ) and the maximum capacity:

$$\tau \text{PCap}_{pgt} \leq \text{PE}_{ipgt} \leq \text{PCap}_{pgt} \quad \forall i, p, g, t \quad (10)$$

The capacity of technology  $p$  in any time period  $t$  is equal to the summation of the existing capacity at the end of the previous period, plus the expansion in capacity carried out in that period ( $\text{PCapE}_{pgt}$ ):

$$\text{PCap}_{pgt} = \text{PCap}_{pgt-1} + \text{PCapE}_{pgt} \quad \forall p, g, t \quad (11)$$

Equation 12 limits the capacity expansions  $\text{PCapE}_{pgt}$  between upper and lower bounds, denoted by  $\underline{\text{PCap}}_p$  and  $\overline{\text{PCap}}_p$ , respectively. This equation makes use of the integer variable  $\text{NP}_{pgt}$

which denotes the number of plants installed in region  $g$  and time period  $t$ .

$$\underline{\text{PCap}}_p \text{NP}_{pgt} \leq \text{PCapE}_{pgt} \leq \overline{\text{PCap}}_p \text{NP}_{pgt} \quad \forall p, g, t \quad (12)$$

Note that the model assumes that a capacity expansion must begin and finish within a time period. In a design problem like the one addressed in the present work, a time period could have a length of one to several years. Hence, the execution of the maximum allowable capacity expansion should always fit within one time period.

The capacity of a storage technology  $s$  in any time period  $t$  is determined from the existing capacity at the end of the previous period and the expansion in capacity in the current period ( $SCapE_{sgt}$ ):

$$SCap_{sgt} = SCap_{sgt-1} + SCapE_{sgt} \quad \forall s, g, t \quad (13)$$

The storage capacity expansions are also limited by lower and upper bounds, as stated in eq 14. Here, the integer variable  $\text{NS}_{sgt}$  accounts for the number of storage facilities installed in region  $g$  and time period  $t$ .

$$\underline{SCap}_s \text{NS}_{sgt} \leq SCapE_{sgt} \leq \overline{SCap}_s \text{NS}_{sgt} \quad \forall s, g, t \quad (14)$$

The materials flows are constrained between lower and upper capacity limits ( $Q_l$  and  $\overline{Q}_l$  respectively):

$$\begin{aligned} Q_l X_{lg'gt} &\leq \sum_{i \in IL(i, l)} Q_{ilgg't} \leq \overline{Q}_l X_{lg'gt} \\ \forall l, t, g, g' (g' \neq g) \end{aligned} \quad (15)$$

In this equation,  $IL(i, l)$  represents the set of allowable combinations between materials  $i$  and suitable transportation modes  $l$ .

**Objective Function.** The model seeks to optimize the economic and environmental performance of the network. The economic objective is represented by the net present value (NPV), whereas the environmental impact is quantified according to LCA principles.

**Net Present Value.** The NPV can be determined from the discounted cash flows ( $CF_t$ ) generated in each of the time intervals  $t$  in which the total time horizon is divided:

$$\text{NPV} = \sum_t \frac{CF_t}{(1 + ir)^{t-1}} \quad (16)$$

In this equation,  $ir$  represents the interest rate. The cash flow that appears in eq 16 is determined from the net earnings  $NE_t$  (i.e., profit after taxes), and the fraction of the total depreciable capital ( $FTDC_t$ ) as follows:

$$CF_t = NE_t - FTDC_t \quad t = 1, \dots, T-1 \quad (17)$$

In the calculation of the cash flow corresponding to the last time period ( $t = T$ ), we assume that part of the total fixed capital investment (FCI) may be recovered at the end of the time horizon. This amount, which represents the salvage value of the network (sv), may vary from one type of industry to another.

$$CF_t = NE_t - FTDC_t + svFCI \quad t = T \quad (18)$$

The net earnings are given by the difference between the incomes ( $Rev_t$ ) and the facility operating (FOC $_t$ ), and transportation cost (TOC $_t$ ), as stated in eq 19:

$$NE_t = (1 - \varphi)(Rev_t - FOC_t - TOC_t) + \varphi DEP_t \quad \forall t \quad (19)$$

In this equation,  $\varphi$  denotes the tax rate. The revenues are determined from the sales of final products and the corresponding

Table 5. Environmental Impact Factors,  $v_b$ 

product	subsystem	unit	GWP100 kg CO <sub>2</sub> eq.	EI99 ecopoints	HH ecopoints	EQ ecopoints	Res ecopoints
sugar cane	Agriculture + Milling	kg sugar cane	-0.2573	0.0746	0.0563	0.0169	0.0014
white sugar	sugar production by technology T1	kg sugar	0.0189	0.0019	0.0014	0.0001	0.0004
white sugar	sugar production by technology T2	kg sugar	0.0227	0.0023	0.0017	0.0001	0.0004
ethanol	ethanol production by any technology	kg ethanol	3.0078	0.0182	0.0171	0.0001	0.0009
sugar cane	transportation by heavy trucks <sup>39</sup>	tkm	0.1364	0.0113	0.0046	0.0009	0.0059
sugar	transportation by medium-sized trucks	tkm	0.1034	0.0079	0.0022	0.0005	0.0052
ethanol	transportation by tank trucks	tkm	0.2681	0.0173	0.0053	0.0012	0.0108

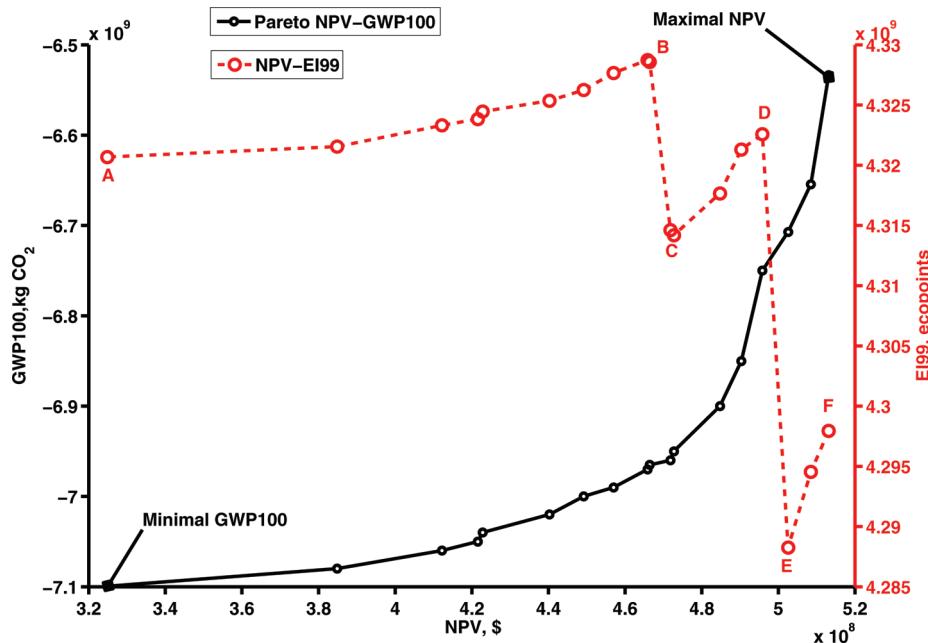


Figure 4. Pareto set of solutions GWP100 vs NPV, and corresponding values of EI99.

prices ( $PR_{igt}$ ):

$$Rev_t = \sum_{i \in SEP(i)} \sum_g DTS_{igt} PR_{igt} \quad \forall t \quad (20)$$

In this equation,  $SEP(i)$  represents the set of materials  $i$  that can be sold. The operating costs are obtained by multiplying the unit production and storage costs ( $UPC_{ipgt}$  and  $USC_{isgt}$ , respectively) with the corresponding production rates and average inventory levels, respectively. This term includes also the disposal cost ( $DC_t$ ):

$$\begin{aligned} FOC_t = & \sum_i \sum_g \sum_{p \in IM(i,p)} UPC_{ipgt} PE_{ipgt} \\ & + \sum_i \sum_g \sum_{s \in IS(i,s)} USC_{isgt} AIL_{isgt} + DC_t \quad \forall t \quad (21) \end{aligned}$$

The disposal cost is a function of the amount of waste generated and landfill tax ( $LT_{igt}$ ):

$$DC_t = \sum_i \sum_g W_{igt} LT_{igt} \quad \forall t \quad (22)$$

The transportation cost includes the fuel ( $FC_t$ ), labor ( $LC_t$ ), maintenance ( $MC_t$ ), and general ( $GC_t$ ) costs:

$$TOC_t = FC_t + LC_t + MC_t + GC_t \quad \forall t \quad (23)$$

The fuel cost is a function of the fuel price ( $FP_{lt}$ ) and fuel usage:

$$FC_t = \sum_{i \in IL(i,l)} \sum_g \sum_{g' \neq g} \sum_l \left[ \frac{2EL_{gg'} Q_{lgg't}}{FE_l TCap_l} \right] FP_{lt} \quad \forall t \quad (24)$$

In eq 24, the fractional term represents the fuel usage, which is determined from the total distance traveled in a trip ( $2EL_{gg'}$ ), the fuel consumption of transport mode  $l$  ( $FE_l$ ) and the number of trips made per period of time ( $Q_{lgg't}/TCap_l$ ). Note that this equation considers that the transportation units operate only between two predefined regions. Furthermore, as shown in eq 25, the labor transportation cost is a function of the driver wage ( $DW_{lt}$ ) and total delivery time (term inside the brackets):

$$LC_t = \sum_{i \in IL(i,l)} \sum_g \sum_{g' \neq g} \sum_l DW_{lt} \left[ \frac{Q_{lgg't}}{TCap_l} \left( \frac{2EL_{gg'}}{SP_l} + LUT_l \right) \right] \quad \forall t \quad (25)$$

The maintenance cost accounts for the general maintenance of the transportation systems, and it is a function of the cost per unit of distance traveled ( $ME_l$ ), and total distance driven:

$$MC_t = \sum_{i \in IL(i,l)} \sum_g \sum_{g' \neq g} \sum_l ME_l \frac{2EL_{gg'} Q_{lgg't}}{TCap_l} \quad \forall t \quad (26)$$

Finally, the general cost includes the transportation insurance, license and registration, and outstanding finances. It can be determined from the general expenses ( $GE_{lt}$ ) and number of transportation units ( $NT_{lt}$ ), as follows:

$$GC_t = \sum_l \sum_{t' \leq t} GE_{lt'} NT_{lt'} \quad \forall t \quad (27)$$

The depreciation term is calculated with the straight-line method, similarly as in other SCM models available in the literature.<sup>8,22</sup>

$$DEP_t = \frac{(1-sv)FCI}{T} \quad \forall t \quad (28)$$

where FCI denotes the total fixed cost investment, which is determined from the capacity expansions made in plants and warehouses as well as the number of transportation units purchased during the entire time horizon as follows:

$$\begin{aligned} FCI = & \sum_p \sum_g \sum_t (\alpha_{pgt}^{Pr} NP_{pgt} + \beta_{pgt}^{Pr} PCapE_{pgt}) \\ & + \sum_s \sum_g \sum_t (\alpha_{sgt}^{St} NS_{sgt} + \beta_{sgt}^{St} SCapE_{sgt}) \\ & + \sum_l \sum_t NT_{lt} \cdot TMC_{lt} \end{aligned} \quad (29)$$

Here, the parameters  $\alpha_{pgt}^{Pr}$ ,  $\beta_{pgt}^{Pr}$  and  $\alpha_{sgt}^{St}$ ,  $\beta_{sgt}^{St}$  are the fixed and variable investment terms corresponding to plants and warehouses, respectively. On the other hand,  $TMC_{lt}$  is the investment cost associated with transportation mode  $l$ . The average number of trucks required by the SC is calculated from the flow rates of materials between regions, the transportation mode availability ( $avl_l$ ), the capacity of a transport container, the average distance traveled between regions, the average speed, and the loading/unloading time, as stated in eq 30:

$$\sum_{t \leq T} NT_{lt} = \sum_{i \in IL(i,l)} \sum_g \sum_{g' \neq g} \sum_t \frac{Q_{ilgg't}}{avl_l TCap_l} \left( \frac{2EL_{gg'}}{SP_l} + LUT_l \right) \quad \forall l \quad (30)$$

An upper limit on the total capital investment can be defined as follows:

$$FCI \leq \overline{FCI} \quad (31)$$

Finally, the model assumes that the total capital investment is divided into several payments of equal amount ( $FTDC_t$ ):

$$FTDC_t = \frac{FCI}{T} \quad \forall t \quad (32)$$

**Environmental Impact.** The main sources of impact associated with the SC operation are the production of the main feedstock, sugar cane, the manufacturing and storage tasks, and the transportation of materials between regions. Mathematically, the inventory of emissions due to the operation of the network can be expressed as a function of some continuous variables of the model. Specifically, the entries of the life cycle inventory can be calculated from the production rates at the plants ( $PE_{ipgt}$ ), and the transportation flows ( $Q_{ilgg't}$ ), as stated in eq 33.

$$\begin{aligned} LCI_b = & \sum_i \sum_g \sum_p \sum_t PE_{ipgt} \omega_{bp}^{Pr} \\ & + \sum_i \sum_g \sum_{g' \neq g} \sum_{l \in IL(i,l)} \sum_t Q_{ilgg't} EL_{gg'} \omega_b^{Tr} \quad \forall b \end{aligned} \quad (33)$$

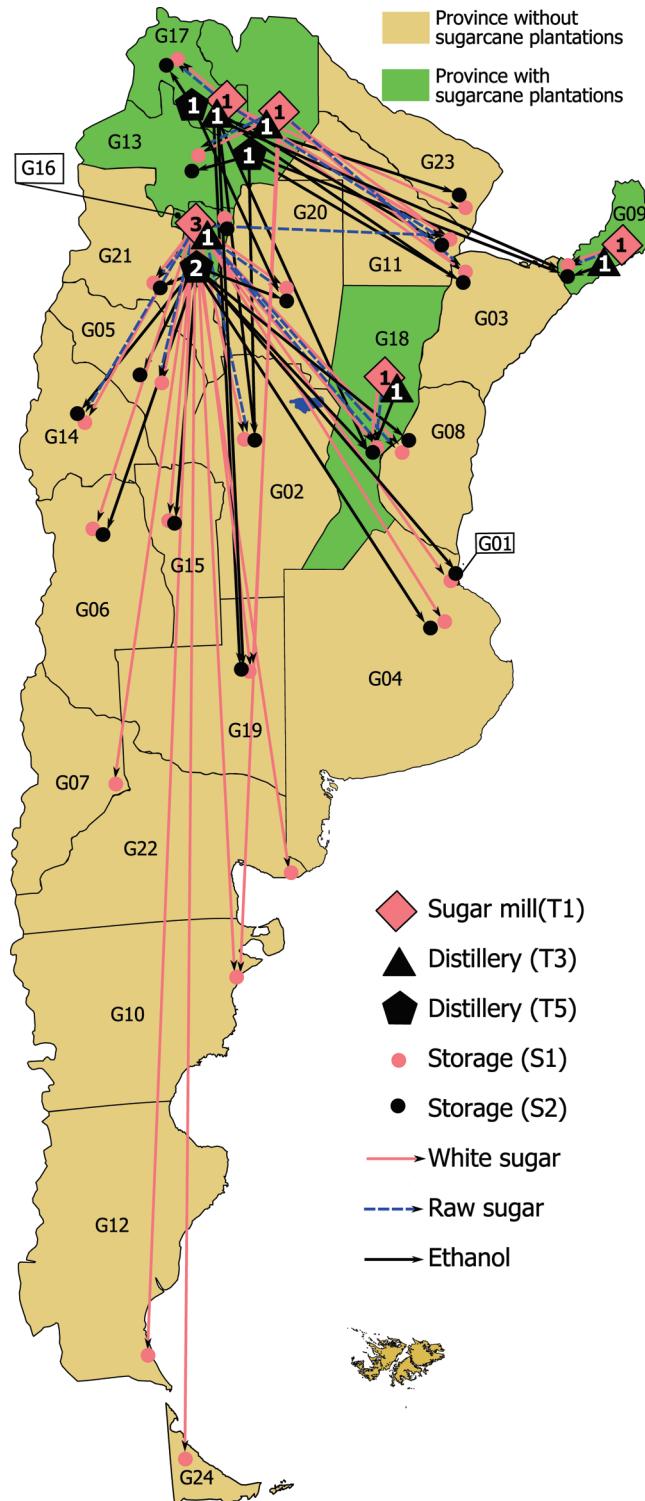


Figure 5. SC configuration of the minimum GWP100 solution.

The first term in eq 33 represents the emissions associated with the manufacturing tasks, which include the agricultural stage, sugar cane milling, sugar manufacturing, ethanol manufacturing, and generation of utilities (i.e., steam and electricity). The second term in eq 33 considers the emissions due to the transportation tasks.  $\omega_{bp}^{Pr}$  and  $\omega_b^{Tr}$  denote the life cycle inventory entries (i.e., emissions released to the environment or resource taken from the ecosystem) associated with

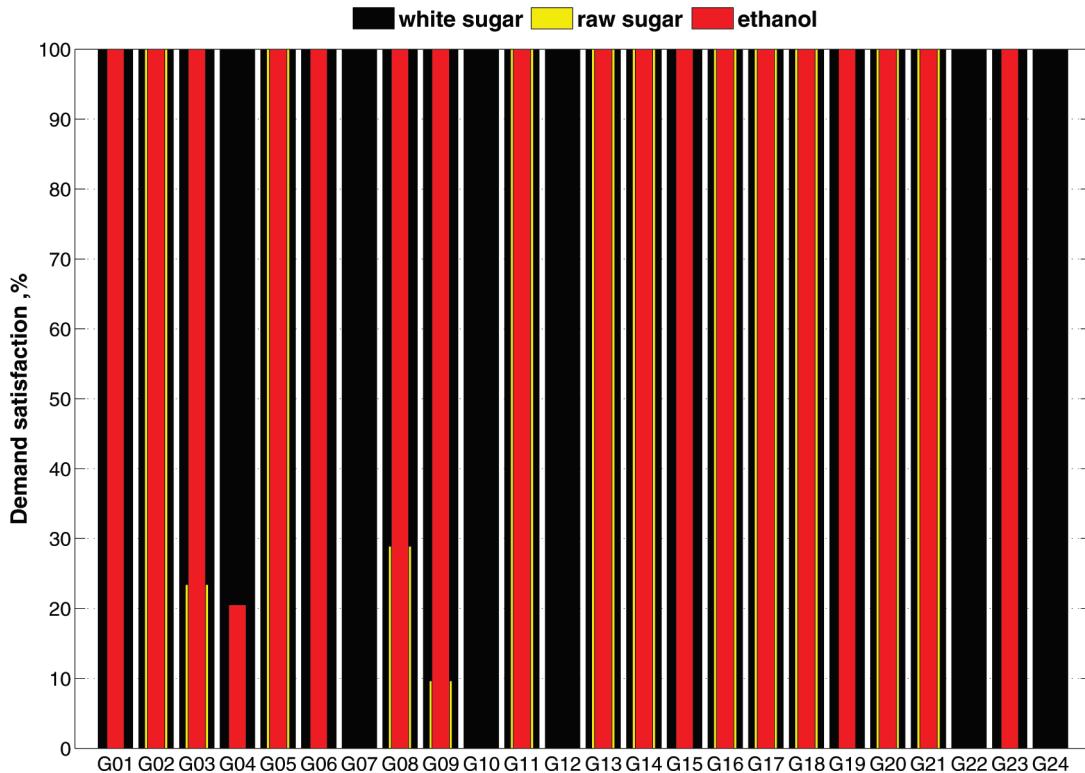


Figure 6. Demand satisfaction level associated with the minimum GWP100 solution.

chemical  $b$  per reference flow of activity. In the manufacturing tasks, the reference flow is one unit of main product produced. For the transportation tasks, the reference flow is one unit of mass transported one unit of distance.

The damage caused is calculated by multiplying the life cycle inventory entries with the corresponding damage factors ( $v_b$ ), as stated in equation eq 34,

$$\text{DAM} = \sum_b v_b \cdot \text{LCI}_b \quad (34)$$

Note that variable DAM is the environmental metric to be minimized, whereas the value of the parameter  $v_b$  is given by the GWP100 and EI99 methodologies.

*Multiobjective Problem.* The overall bi-MILP formulation can be expressed in compact form as follows:

$$(M) \quad \begin{aligned} & \min_{x, X, N} \{-\text{NPV}(x, X, N); \text{DAM}(x, X, N)\} \\ & \text{s.t. constraints 1-34} \\ & x \in \mathbb{R}, \quad X \in \{0, 1\}, \quad N \in \mathbb{Z}^+ \end{aligned}$$

Here,  $x$  generically denotes the continuous variables of the problem (capacity expansions, production rates, inventory levels, and materials flows),  $X$  represents the binary variables (i.e., establishment of transportation links), and  $N$  are the integer variables denoting the number of plants, storage facilities, and transport units of each type selected. The solution to this problem is given by a set of Pareto alternatives representing the optimal trade-off between the objectives considered in the analysis.

In this work, the Pareto solutions are determined via the  $\varepsilon$ -constraint method,<sup>43</sup> which entails solving a set of instances of the following single-objective problem M1 for different values of

the auxiliary parameter  $\varepsilon$ :

$$(M1) \quad \begin{aligned} & \min_{x, X, N} \{-\text{NPV}(x, X, N)\} \\ & \text{s.t. constraints 1-34} \\ & \text{DAM}(x, X, N) \leq \varepsilon \\ & \underline{\varepsilon} \leq \varepsilon \leq \bar{\varepsilon} \\ & x \in \mathbb{R}, \quad X \in \{0, 1\}, \quad N \in \mathbb{Z}^+ \end{aligned}$$

where the lower and upper limits within which the epsilon parameter must fall (i.e.,  $\varepsilon \in [\underline{\varepsilon}, \bar{\varepsilon}]$ ) are obtained from the optimization of each separate scalar objective:

$$(M1a) \quad (\bar{x}\bar{X}\bar{N}) = \arg \min_{x, X, N} \{\text{DAM}(x, X, N)\} \\ \text{s.t. constraints 1-34} \\ x \in \mathbb{R}, \quad X \in \{0, 1\}, \quad N \in \mathbb{Z}^+$$

which defines  $\underline{\varepsilon} = \text{DAM}(\bar{x}\bar{X}\bar{N})$  and

$$(M1b) \quad (\hat{x}\hat{X}\hat{N}) = \arg \min_{x, X, N} \{-\text{NPV}(x, X, N)\} \\ \text{s.t. constraints 1-34} \\ x \in \mathbb{R}, \quad X \in \{0, 1\}, \quad N \in \mathbb{Z}^+$$

which defines  $\bar{\varepsilon} = \text{DAM}(\hat{x}\hat{X}\hat{N})$ .

## CASE STUDY

We illustrate the capabilities of the proposed approach through a case study based on the sugar cane industry of Argentina. The geographic scope of the problem has been defined according to the administrative divisions of the country.

We therefore consider 24 provinces with an associated sugar and ethanol demand. The data employed in the analysis are provided in the Appendix section at the end of the article. The parameters used in the calculations of the global warming potential (GWP100), and Eco-Indicator 99 (EI99) are shown in Table 5.

The bicriteria model was written in GAMS<sup>44</sup> and solved with the MILP solver CPLEX 11.0 on a HP Compaq DCS850 desktop PC with an AMD Phenom 8600B, 2.29 GHz triple-core processor, and 2.75 Gb of RAM. Particularly, we generated two different Pareto sets: NPV versus GWP100, and NPV versus EI99. Each instance of problem M1 was solved to global optimality. The resulting optimization model contains 24 296 equations, 23 790 continuous variables, and 5481 discrete variables. The CPU time spent to find a single Pareto solution varies between 282 and 25 615 s. In the sections that follow, we provide a detailed analysis of the solutions found.

**Pareto Set Global Warming Potential versus Net Present Value.** We first determine the Pareto set global warming potential versus net present value. Figure 4 shows the obtained results. The solid line represents the Pareto points that trade-off GWP100 and NPV, whereas the dashed line shows the corresponding values of EI99 for each Pareto solution. That is, we show here two projections of the Pareto solutions GWP100 versus NPV, one projection onto the subspace GWP100 versus NPV (primary *y* axis), and another one onto the subspace EI99 versus NPV (secondary *y* axis). As observed, reductions in CO<sub>2</sub> emissions can only be achieved at the expense of compromising the benefit. As seen, the NPV increases from  $\$3.2 \times 10^8$  to  $\$5.1 \times 10^8$ , that is, about 58% from the minimum impact solution to the maximum NPV one. Such an economical gain entails a less significant rise in the CO<sub>2</sub> emissions (8%, from  $-7.1 \times 10^9$  kg CO<sub>2</sub> to  $-6.5 \times 10^9$  kg CO<sub>2</sub>).

Note that each point of the Pareto set represents a different SC configuration operating under a set of specific conditions. Figure 5 shows the SC configurations corresponding to the minimum environmental impact solution in Figure 4. In this solution, the SC includes seven sugar mills utilizing technology T1, five distilleries, T3, that convert molasses into ethanol, and four distilleries, T5. All these production facilities are located in five provinces that have sugar cane plantations. The consumption of sugar cane in this solution is 100% (i.e., all the available sugar cane is consumed). This results in great reductions of CO<sub>2</sub> emissions, mainly because sugar cane cultivation is carbon negative; that is, it has a negative overall contribution to global warming. The choice of the tandem T1–T3 in the minimum impact solution is motivated by their lower values of GWP100, as compared to T2–T4.

Figure 6 shows the demand satisfaction level for the minimum GWP100 solution. As observed, the white sugar and ethanol demands are fully satisfied only in the provinces that have sugar cane plantations as well as in their neighboring provinces. Misiones (G09) and Santa Fe (G18) do not have enough sugar cane to fulfill their internal demand, and for this reason they import ethanol and sugar from northwestern provinces. The capital investment in this solution is  $\$1.8 \times 10^9$ .

Figure 7 shows the topology of the maximum NPV alternative. As observed, this solution leads to a more centralized network. Three sugar mills T2, one distillery T4, and three distilleries T5 are located in the northwest of Argentina. In this solution, not all the available sugar cane is processed (98.6% in this case versus 100% in the minimum impact one). In fact, the model avoids

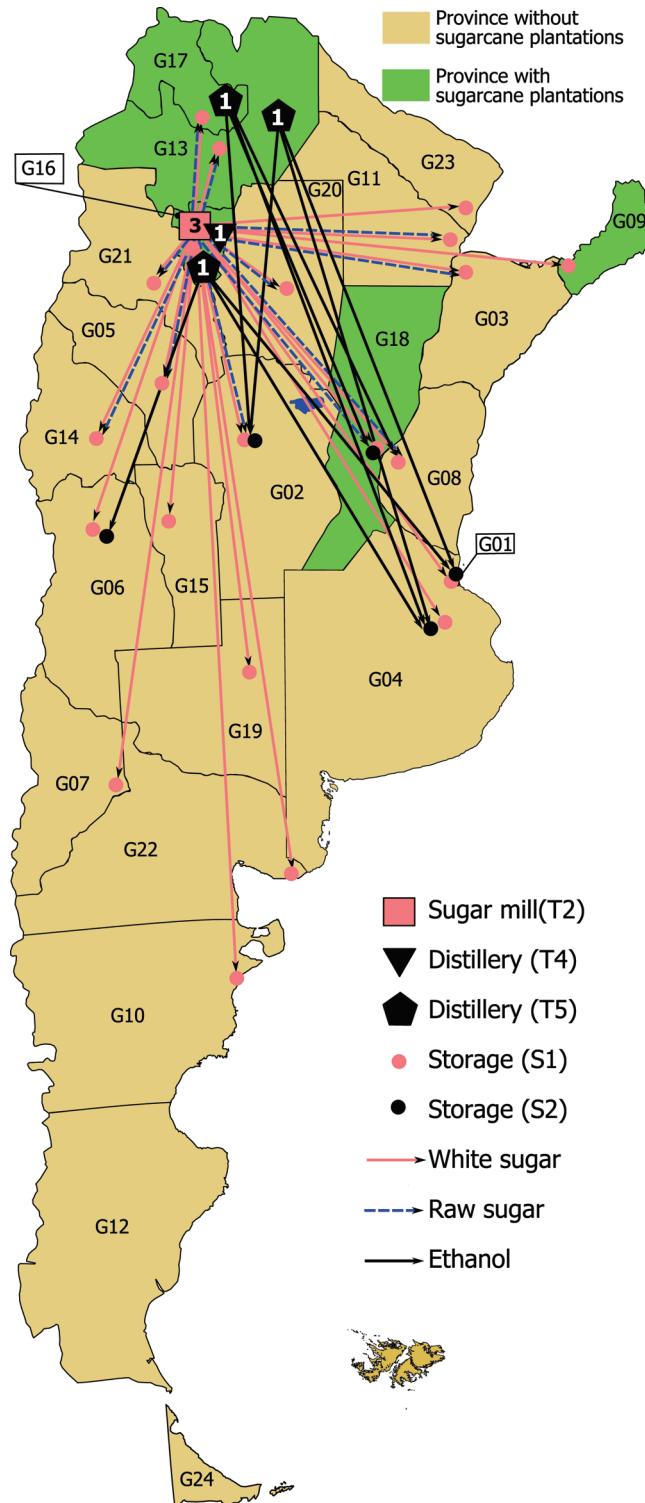


Figure 7. SC configuration of the maximum NPV solution.

installing production facilities in Misiones (G09) and Santa Fe (G18). The selection of technologies T2–T4 is explained by their larger ethanol yield. Particularly, T1–T3 can convert 100 kg of sugar cane into 1.23 kg of ethanol, whereas the pair T2–T4 produces 2.24 kg of ethanol from the same amount of sugar cane. Storages for liquid products are only established in provinces with high ethanol demand, even if they are far away from the manufacturing plants. In contrast, in the minimum GWP100

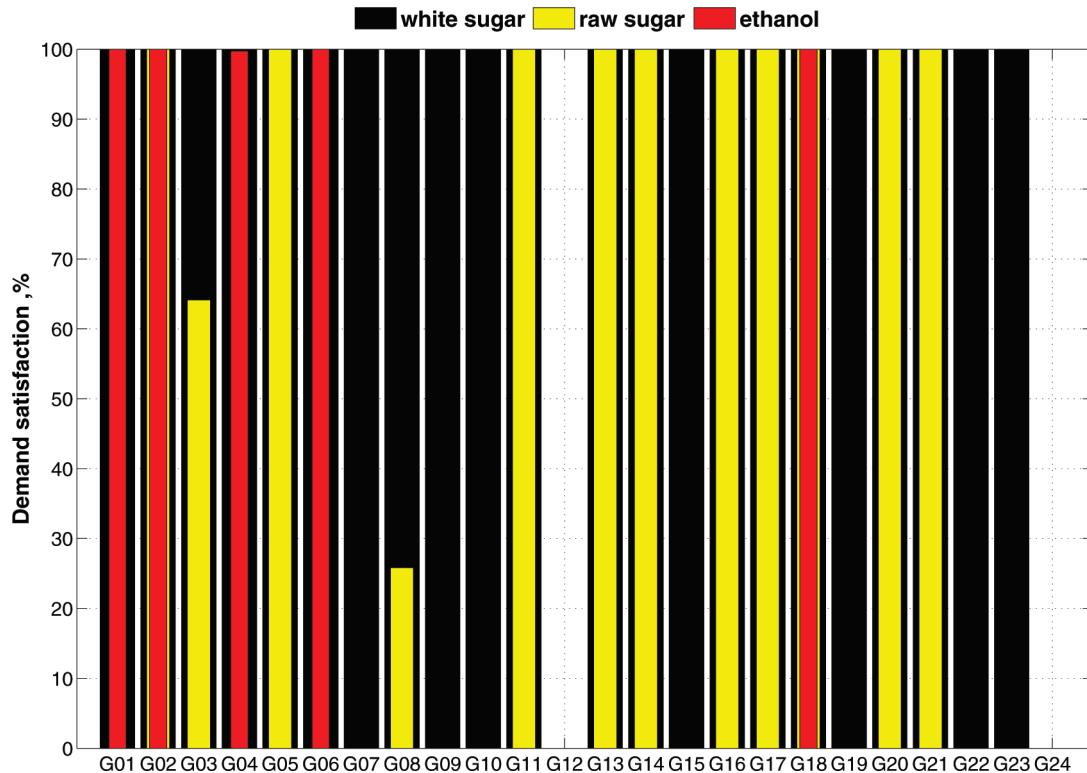


Figure 8. Demand satisfaction level associated with the maximum NPV solution.

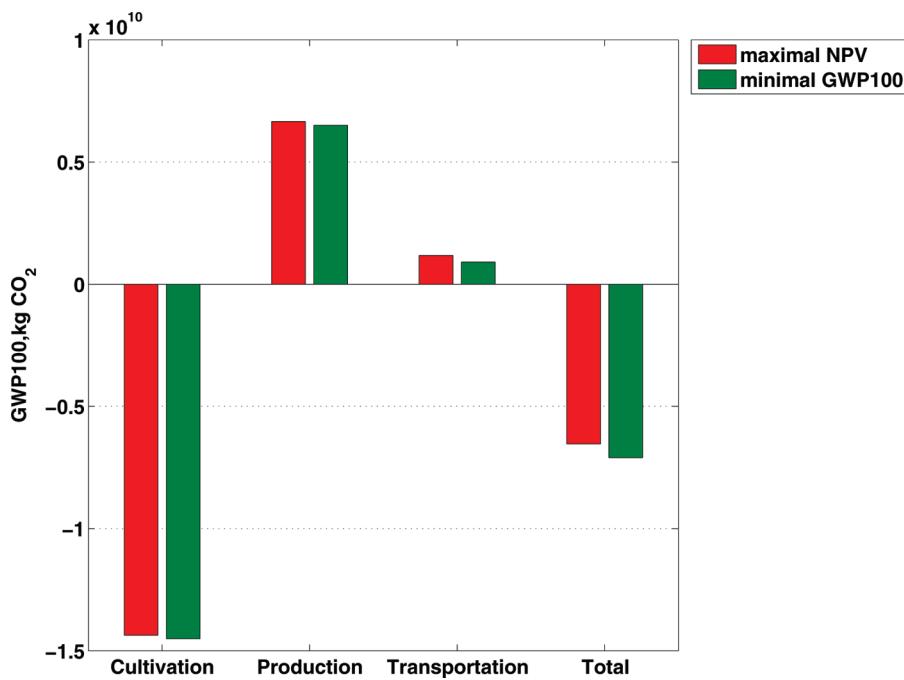


Figure 9. Contribution of different SC stages to the GWP100 for the extreme solutions.

solution, storage facilities are opened as close as possible to the plants in order to minimize the CO<sub>2</sub> emissions associated with the transportation tasks. The capital investment of the maximum NPV solution is  $\$1.4 \times 10^9$ .

The demand satisfaction level is shown in Figure 8. As observed, the most profitable solution satisfies less demand than

the minimum environmental impact one. As an example, note that white sugar is delivered to regions G12 and G24 in the minimum impact solution, whereas in the maximum NPV solution the demand of these provinces is not covered.

Three intervals with different strategic and planning decisions can be clearly distinguished in the Pareto set. The interval AB

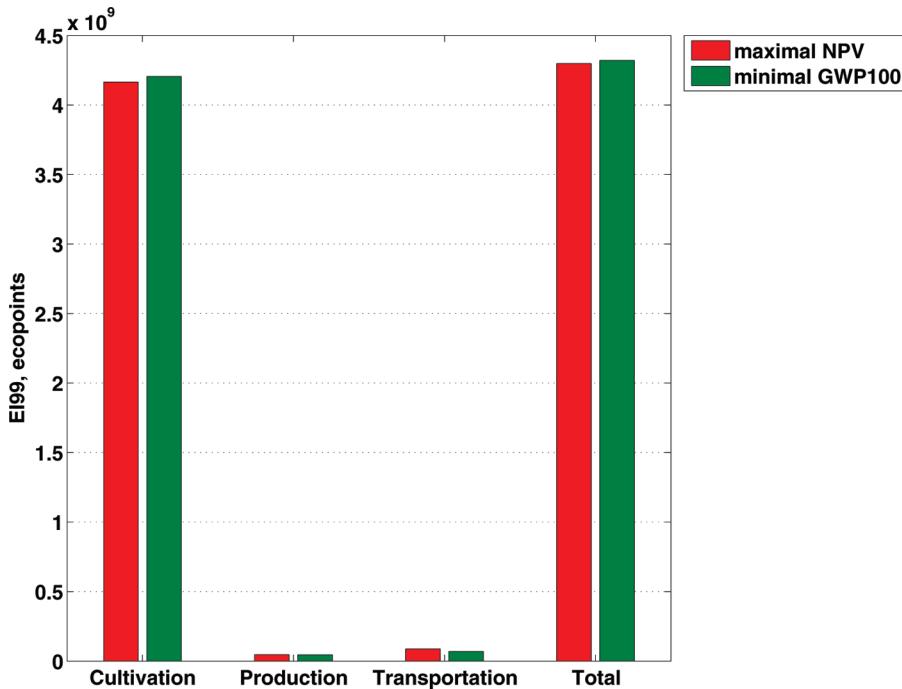


Figure 10. Contribution of different SC stages to the EI99 for the extreme solutions.

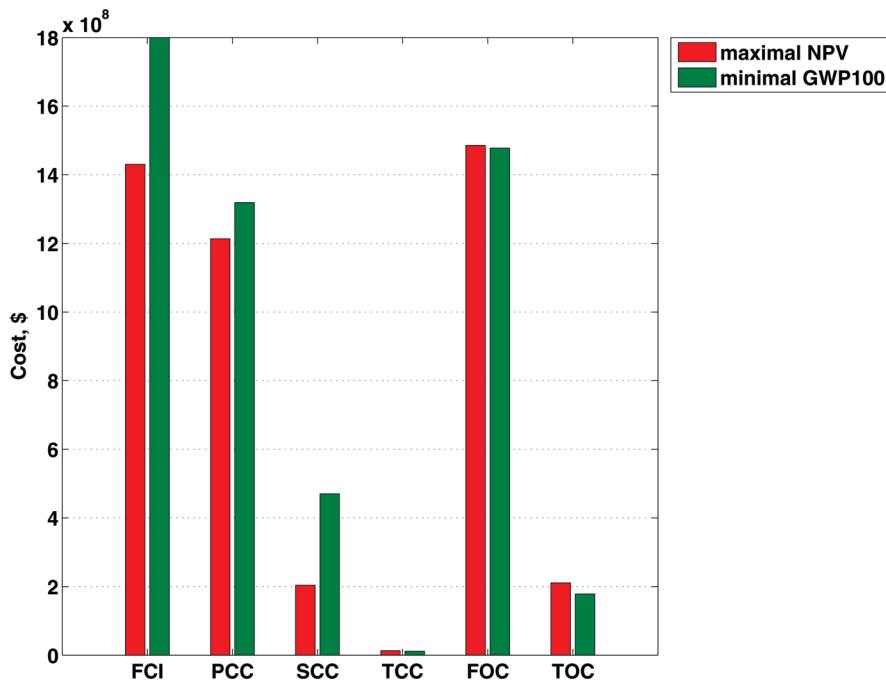


Figure 11. Breakdown of total cost into facility capital investment (FCI), plant capital cost (PCC), storage capital cost (SCC), transportation capital cost (TCC), facility operating cost (FOC) and transportation operating cost (TOC) for the extreme solutions.

entails solutions with decentralized SCs that consume all the available sugar cane and produce ethanol and sugar via technologies T1, T3, and T5. The solutions within this region differ from each other in the planning decisions. The solutions in the interval CD also show decentralized configurations with plants utilizing technologies T1, T3, and T5. The main difference between solutions lying in the interval AB and those in CD is the absence of production facilities in region

G09. Solutions from the last interval EF show SC configurations that combine T1–T3 with T2–T4. All the solutions in the interval EF avoid the establishment of production plants in regions G09 and G18.

It is interesting to note that reducing the CO<sub>2</sub> emissions has the effect of increasing other environmental impacts. Particularly, the minimum GWP100 solution leads to larger EI99 values than the maximum NPV one. These results are explained

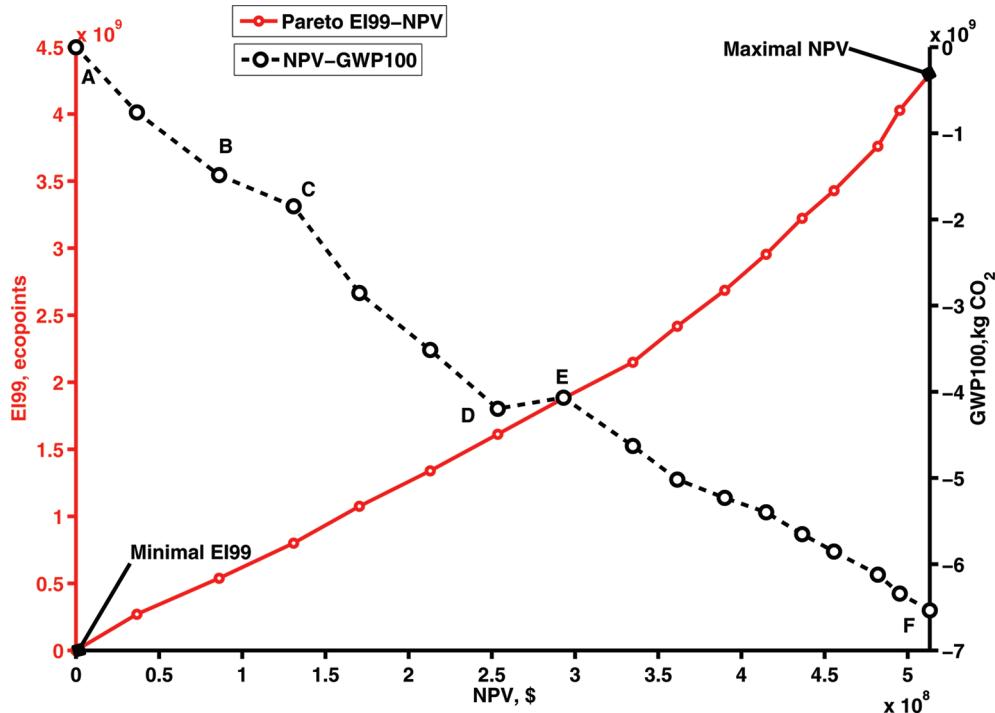


Figure 12. Pareto set of solutions EI99 versus NPV, and corresponding values of GWP100.

Table 6. Product Demand, t/yr

name of province	associated subregion	product form		
		white sugar	raw sugar	ethanol
Buenos Aires	G01	76 614.92	38 307.46	84 276.41
Córdoba	G02	84 126.19	42 063.09	92 538.81
Corrientes	G03	25 438.16	12 719.08	27 981.97
La Plata	G04	379 268.90	189 634.45	417 195.79
La Rioja	G05	9 714.57	4 857.29	10 686.03
Mendoza	G06	43 565.35	21 782.67	47 921.88
Neuquén	G07	13 720.58	6 860.29	15 092.64
Entre Ríos	G08	31 547.32	15 773.66	34 702.05
Misiones	G09	27 140.71	13 570.36	29 854.78
Chubut	G10	11 517.28	5 758.64	12 669.00
Chaco	G11	26 439.66	13 219.83	29 083.63
Santa Cruz	G12	5 708.56	2 854.28	6 279.42
Salta	G13	30 746.12	15 373.06	33 820.73
San Juan	G14	17 526.29	8 763.14	19 278.92
San Luis	G15	11 016.52	5 508.26	12 118.18
Tucumán	G16	37 155.73	18 577.87	40 871.31
Jujuy	G17	17 125.69	8 562.84	18 838.26
Santa Fe	G18	81 121.68	40 560.84	89 233.85
La Pampa	G19	8 412.62	4 206.31	9 253.88
Santiago del Estero	G20	21 732.60	10 866.30	23 905.86
Catamarca	G21	8 612.92	4 306.46	9 474.21
Río Negro	G22	15 022.53	7 511.27	16 524.79
Formosa	G23	13 520.28	6 760.14	14 872.31
Tierra del Fuego	G24	3 204.81	1 602.40	3 525.29

by the environmental impact associated with the agriculture of sugar cane. As mentioned before, the main environmental advantage of the sugar cane plant is that it consumes more CO<sub>2</sub> than the one released during its processing. On the other hand, its cultivation causes other negative effects, mainly in terms of land use and emissions of inorganic compounds to air. According to the EI99 methodology, the negative effects

compensate for the positive ones, so in general terms, sugar cane plantations lead to positive impacts.

Figure 9 shows the contribution of each source of impact (i.e., cultivation, production, and transportation) to the GWP100 for the extreme Pareto solutions. The cultivation of sugar cane shows in both cases the largest contribution to the total impact. Note that sugar cane cultivation has a large negative GWP100 that offsets the positive impacts associated with the transportation and production tasks.

Figure 10 shows a breakdown of the EI99 for the extreme solutions. As observed, the cultivation is the main source of overall impact (measured through the EI99) in both cases. It is interesting to notice that the impact due to transportation and production tasks is rather small in comparison with that associated with the cultivation tasks.

A breakdown of the total cost is given in Figure 11. As observed, a large percentage of the capital investment corresponds to the production facilities. In the minimum GWP100 solution, the total capital investment is larger than in the maximum NPV one. This is due to the larger number of production and storage facilities associated with the minimum GWP100 solution. On the other hand, the maximum NPV solution leads to larger transportation capital and operating cost, since it involves a more centralized network.

**Pareto set Eco-indicator 99 versus Net Present Value.** We next generate the Pareto curve Eco-indicator 99 versus net present value. The results are shown in Figure 12. The solid curve of the figure shows the projections of the Pareto points onto the subspace EI99 versus NPV, whereas the dashed line represents projections onto the subspace GWP100 versus NPV.

Again, the environmental impact (EI99) is reduced at the expense of compromising the NPV. Note that the minimum environmental impact solution avoids the establishment of any type of facility. As observed in Table 5, all the activities carried out

**Table 7.** Distances between Subregions, km

	G01	G02	G03	G04	G05	G06	G07	G08	G09	G10	G11	G12	G13	G14	G15	G16	G17	G18	G19	G20	G21	G22	G23	G24
G01	0	711	933	60	1 167	1 080	1 178	511	1 008	1 379	953	2 542	1 542	1 140	800	1 229	1 565	484	607	1 070	1 122	948	1 098	3 162
G02	711	0	900	768	460	1 153	360	1 118	1 524	880	2 638	844	600	420	597	867	340	667	439	433	1 208	1 031	3 258	
G03	933	900	0	990	1 024	1 490	1 913	573	335	2 206	20	3 369	830	1 460	1 190	794	853	540	1 388	635	857	1 774	186	3 989
G04	60	768	990	0	1 224	1 137	1 159	568	1 065	1 371	1 010	2 533	1 599	1 197	857	1 286	1 622	541	664	1 127	1 173	924	1 236	3 153
G05	1 167	460	1 024	1 224	0	612	1 427	820	1 333	1 872	1 007	3 087	704	355	559	382	727	800	1 015	389	171	1 565	1 139	3 707
G06	1 080	680	1 490	1 137	612	0	815	952	1 710	1 628	1 470	2 783	1 311	166	264	872	1 329	930	789	1 007	725	1 342	1 600	3 403
G07	1 178	1 153	1 913	1 159	1 427	815	0	1 413	2 075	746	1 880	1 909	1 997	981	890	1 581	2 020	1 373	535	1 618	1 536	557	2 020	2 529
G08	511	360	573	568	820	952	1 413	0	758	1 715	590	2 887	1 107	950	691	794	1 130	30	855	635	803	1 252	746	3 507
G09	1 008	1 118	335	1 065	1 333	1 710	2 075	758	0	2 336	332	3 511	1 142	1 708	1 449	1 086	1 165	785	1 518	927	1 179	1 896	508	4 131
G10	1 379	1 524	2 206	1 371	1 872	1 628	746	1 715	2 356	0	2 236	1 172	2 308	1 705	1 382	2 107	2 331	1 685	857	1 986	1 900	809	2 450	1 792
G11	953	880	20	1 010	1 007	1 470	1 880	590	332	2 236	0	3 388	813	1 460	1 190	774	833	540	1 368	618	820	1 756	173	4 008
G12	2 542	2 638	3 369	2 533	3 087	2 783	1 909	2 887	3 511	1 172	3 388	0	3 482	2 868	2 545	3 192	3 505	2 850	2 020	3 070	3 167	1 952	3 593	620
G13	1 542	844	830	1 599	704	1 311	1 997	1 107	1 142	2 308	813	3 482	0	1 150	1 264	310	90	1 077	1 462	472	533	2 066	959	4 102
G14	1 140	600	1 460	1 197	355	166	981	950	1 708	1 705	1 460	2 868	1 150	0	320	708	1 163	920	848	840	497	1 509	1 540	3 488
G15	800	420	1 190	857	559	264	890	691	1 449	1 382	1 190	2 545	1 264	320	0	838	1 287	660	525	859	674	1 087	1 345	3 165
G16	1 229	597	794	1 286	382	872	1 581	794	1 086	2 107	774	3 192	310	708	838	0	328	764	1 257	164	221	1 803	925	3 812
G17	1 565	867	853	1 622	727	1 329	2 020	1 130	1 165	2 331	833	3 505	90	1 163	1 287	328	0	1 092	1 485	490	563	2 095	921	4 125
G18	484	340	540	541	800	930	1 373	30	785	1 685	540	2 850	1 077	920	660	764	1 092	0	828	605	777	1 218	709	3 470
G19	607	667	1 388	664	1 015	789	535	855	1 518	857	1 368	2 020	1 462	848	525	1 257	1 485	828	0	1 129	1 065	580	1 492	2 640
G20	1 070	439	635	1 127	389	1 007	1 618	635	927	1 986	618	3 070	472	840	859	164	490	605	1 129	0	234	1 669	751	3 690
G21	1 122	433	857	1 173	171	725	1 536	803	1 179	1 900	820	3 167	533	497	674	221	563	777	1 065	234	0	1 645	985	3 787
G22	948	1 208	1 774	924	1 565	1 342	557	1 252	1 896	809	1 756	1 952	2 066	1 509	1 087	1 803	2 095	1 218	580	1 669	1 645	0	1 922	2 572
G23	1 098	1 031	186	1 236	1 139	1 600	2 020	746	508	2 450	173	3 593	959	1 540	1 345	925	921	709	1 492	751	985	1 922	0	4 213
G24	3 162	3 258	3 989	3 153	3 707	3 403	2 529	3 507	4 131	1 792	4 008	620	4 102	3 488	3 165	3 812	4 125	3 470	2 640	3 690	3 787	2 572	4 213	0

**Table 8.** Sugarcane Capacity, t/year

province	capacity
Tucumán	12 220 000
Jujuy	4 324 000
Salta	2 068 000
Santa Fe	125 960
Misiones	62 040

**Table 9.** Minimum and Maximum Production Capacities of Each Technology (tonnes of Main Product Per Year)

	technologies				
	T1	T2	T3	T4	T5
minimum production capacity	30 000	30 000	10 000	10 000	10 000
maximum production capacity	350 000	350 000	300 000	300 000	300 000

**Table 10.** Parameters Used to Evaluate the Capital Cost for Different Production Technologies

	$\alpha_{pgt}^{Pr}$ (\$)	$\beta_{pgt}^{Pr}$ (\$·yr/t)
T1	5,350,000	535
T2	5,350,000	535
T3	7,710,000	771
T4	7,710,000	771
T5	9,070,000	907

**Table 11.** Parameters Used to Evaluate the Capital Cost for Different Storage Technologies

	$\alpha_{sgt}^{St}$ (\$)	$\beta_{sgt}^{St}$ (\$·yr/t)
S1	1,220,000	122
S2	18,940,000	1 894

in the SC lead to positive impacts. Hence, the minimum EI99 is achieved when no facilities are opened. Similarly, as in the previous case, we identify three main intervals in the Pareto set. Within interval AB, the SC produces ethanol and sugar via technologies T1 and T3, and the plants are situated in Tucumán (G16). Until point B, ethanol is consumed by Tucumán and not transported to other provinces. In the solutions placed after point B, the production rate of ethanol exceeds the demand of this province. Because of this, the SC begins to export ethanol to the neighboring provinces. Finally, the shift from technologies T1–T3 to T2–T4 takes place between points D and F.

## CONCLUSIONS

This work has addressed the optimal design and planning of SCs of the sugar cane industry with economic and environmental concerns. The design task was formulated as a bicriterion MILP that seeks to maximize simultaneously the NPV and life cycle environmental performance of the network. The environmental impact was measured over the entire life cycle of the process by applying two LCA-based methodologies: the Eco-indicator 99 and CML.

The capabilities of the proposed modeling framework and solution strategy were illustrated through a case study based on a

**Table 12.** Parameters Used to Calculate the Capital and Operating Cost for Different Transportation Modes

	heavy truck	medium truck	tanker truck
average speed (km/h)	55	60	65
capacity (ton per trip)	30	25	20
availability of transportation mode (h/d)	18	18	18
cost of establishing transportation mode (\$)	30,000	30,000	30,000
driver wage (\$/h)	10	10	10
fuel economy (km/L)	5	5	5
fuel price (\$/L)	0.85	0.85	0.85
general expenses (\$/d)	8.22	8.22	8.22
load/unload time of product (h/trip)	6	6	6
maintenance expenses (\$/km)	0.0976	0.0976	0.0976

real scenario. The Pareto solutions provide valuable insight into the design problem and suggest process alternatives leading to environmental improvements. Particularly, it was clearly shown how significant environmental savings can be attained by properly adjusting the operating conditions and topology of the SC. Numerical results indicate also that there is a conflict not only between the economic and environmental performance, but also between the LCA-based environmental metrics considered in the optimization problem.

Our tool has been devised to assist authorities in the analysis of strategic policies in the field of agro-industries and energy. Future work will focus on adding new features to the model, such as the option to import and export sugar and bioethanol, and expand the agricultural areas.

## APPENDIX. DATA FOR THE CASE STUDY

The regions considered in the analysis and associated demand are shown in Table 6. For the sake of simplicity, we assume that the demand and prices are constant along the time horizon. The prices for white sugar, raw sugar, and ethanol are equal to 537, 375, and 860 \$/t, respectively. Distances between regions have been determined considering the capitals of the corresponding provinces and the main roads connecting these cities. These data are listed in Table 7. The length of the time horizon is 4 years. We assume that each region has an associated sugar cane crop capacity. Particularly, sugar cane plantations are situated in five Argentine provinces, whose production capacities are shown in Table 8. The minimum and maximum production capacities of each technology are listed in Table 9. The minimum and maximum storage capacities for liquid and solid materials are assumed to be 200 and 2 billion tonnes, respectively. The minimum desired percentage of the available installed capacity ( $\tau$ ) has been fixed to zero, and the storage period ( $\sigma$ ) is equal to 10 days.

The upper limit on the fixed capital investment has been set to  $10^9$  \$. Fixed and variable investment coefficients for different production and storage modes are listed in Table 10 and Table 11, respectively. Unit production cost for sugar and ethanol are equal to 265 and 317 \$/t, respectively. The unit storage cost is 0.365 \$(/t yr) for all types of materials. The parameters used to calculate the capital and operating cost for different transportation modes can be found in Table 12. The

minimum flow rate of each transportation mode is assumed to be equal to the minimum capacity of the corresponding transportation mode (see Table 12), whereas the maximum flow rates for heavy trucks, medium trucks, and tanker trucks are 6.25, 6.25, and 6.00 million tonnes per year, respectively. The tax rate ( $\varphi$ ), salvage value (sv), and interest rate (ir) are 0.3, 0.2, and 0.1, respectively. Finally, the landfill tax is equal to 0.1 \$/t for all types of reliquid residues (vinasses).

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## NOTATION

### Indices

$b$  = chemical specie in the inventory table

$g$  = regions

$i$  = materials

$l$  = transportation modes

$p$  = manufacturing technologies

$s$  = storage technologies

$t$  = time periods

### Sets

$IL(i,l)$  = set of ordered pairs that link materials  $i$  to transport modes  $l$

$IM(i,p)$  = set of ordered pairs that link main products  $i$  to technologies  $p$

$IS(i,s)$  = set of ordered pairs that link materials  $i$  to storage technologies  $s$

$SEP(i)$  = subset of products  $i$  that can be sold

### Parameters

$\alpha_{pgt}^{Pr}$  = fixed investment coefficient for technology  $p$

$\alpha_{sgt}^{St}$  = fixed investment coefficient for storage technology  $s$

$\beta_{pgt}^{Pr}$  = variable investment coefficient for technology  $p$

$\beta_{sgt}^{St}$  = variable investment coefficient for storage technology  $s$

$\varepsilon$  = auxiliary boundary for the  $\varepsilon$ -constraint method

$\rho_{pi}$  = material balance coefficient associated with material  $i$  and technology  $p$

$\sigma$  = storage period

$\tau$  = minimum desired percentage of the available installed capacity that must be utilized

$v_b$  = damage factor associated to chemical specie  $b$

$\varphi$  = tax rate

$\omega_{bp}^{Pr}$  = life cycle environmental burden associated to chemical  $b$  (production stage)

$\omega_b^{Tr}$  = life cycle environmental burden associated to chemical  $b$  (transportation stage)

$avl_l$  = availability of transportation mode  $l$

$CapCrop_{gt}$  = total capacity of sugar cane plantations in region  $g$  in time  $t$

$DW_{lt}$  = driver wage

$EL_{gg'}$  = distance between  $g$  and  $g'$

$\overline{FCI}$  = upper limit on the capital investment

$FE_l$  = fuel consumption of transport mode  $l$

$FP_{lt}$  = fuel price

$GE_{lt}$  = general expenses of transportation mode  $l$

$ir$  = interest rate

$LT_{igt}$  = landfill tax in period  $t$

$LUT_l$  = loading/unloading time of transportation mode  $l$

$ME_l$  = maintenance expenses of transportation mode  $l$

$PCap_p$  = maximum capacity of technology  $p$

$PCap_p$  = minimum capacity of technology  $p$

$PR_{igt}$  = prices of final products

$\overline{Q}_l$  = maximum capacity of transportation mode  $l$

$Q_l$  = minimum capacity of transportation mode  $l$

$SCap_s$  = maximum capacity of storage technology  $s$

$SCap_s$  = minimum capacity of storage technology  $s$

$SD_{igt}$  = actual demand of product  $i$  in region  $g$  in time  $t$

$SP_l$  = average speed of transportation mode  $l$

$sv$  = salvage value

$T$  = number of time intervals

$TCap_l$  = capacity of transportation mode  $l$

$TMC_{lt}$  = cost of establishing transportation mode  $l$  in period  $t$

$UPC_{ipgt}$  = unit production cost

$USC_{isgt}$  = unit storage cost

### Variables

$AIL_{igt}$  = average inventory level of product  $i$  in region  $g$  in period  $t$

$CF_t$  = cash flow in time period  $t$

$DAM$  = environmental damage (expressed in GWP100 or EI99)

$DC_t$  = disposal cost in time period  $t$

$DEP_t$  = depreciation in time period  $t$

$DTS_{igt}$  = amount of material  $i$  delivered in region  $g$  and period  $t$

$FC_t$  = fuel cost

$FCI$  = fixed capital investment

$FOC_t$  = facility operating cost in time period  $t$

$FTDC_t$  = fraction of the total depreciable capital in time period  $t$

$GC_t$  = general cost

$LC_t$  = labor cost

$LCI_b$  = life cycle inventory entry of chemical  $b$

$MC_t$  = maintenance cost

$NE_t$  = net earnings in time period  $t$

$NP_{pgt}$  = number of plants with technology  $p$  established in region  $g$  and time period  $t$

$NPV$  = net present value

$NS_{sgt}$  = number of storages with storage technology  $s$  established in region  $g$  and time period  $t$

$NT_{lt}$  = number of transportation units  $l$

$PCap_{pgt}$  = existing capacity of technology  $p$  in region  $g$  and time period  $t$

$PCapE_{pgt}$  = capacity expansion of technology  $p$  in region  $g$  and time period  $t$

$Q_{ilgg'}$  = flow rate of material  $i$  transported by mode  $l$  from region  $g$  to region  $g'$  in time period  $t$

$Rev_t$  = revenue in time  $t$

$SCap_{sgt}$  = capacity of storage  $s$  in region  $g$  and time period  $t$

$SCapE_{sgt}$  = expansion of the existing capacity of storage  $s$  in region  $g$  and time period  $t$

$ST_{isgt}$  = total inventory of material  $i$  in subregion  $g$  stored by technology  $s$  in time period  $t$

$TOC_t$  = transport operating cost in time period  $t$

- $PE_{ipgt}$  = production rate of material  $i$  associated with technology  $p$  established in region  $g$  and time period  $t$
- $PT_{igt}$  = total production rate of material  $i$  in region  $g$  and time period  $t$
- $PU_{igt}$  = purchases of material  $i$  in region  $g$  and time period  $t$
- $X_{lgg'}$  = binary variable (1 if a transportation link is established between regions  $g$  and  $g'$ , 0 otherwise)
- $W_{igt}$  = amount of wastes  $i$  generated in region  $g$  and time period  $t$

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