UNIVERSITAT ROVIRA I VIRGILI

DEVELOPMENT OF ADVANCED MATHEMATICAL PROGRAMMING METHODS FOR SUPPLY CHAIN MANAGEMENT

Andrey Kostin

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DOCTORAL THESIS

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Supervised by: Dr. **Laureano Jiménez Esteller**
Dr. **Gonzalo Guillén Gosálbez**

Department of Chemical Engineering
SUSCAPE Research Group

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UNIVERSITAT ROVIRA I VIRGILI

Departament d' Enginyeria Química Av. Països Catalans, 26

Campus Sescelades

43007 Tarragona (Spain)

Tel.: +34 977 55 9603

Fax: +34 977 55 9621

Gonzalo Guillén Gosálbez and Laureano Jiménez Esteller, associate professors in the Department of Chemical Engineering,

CERTIFY:

That the present study, entitled "Development of advanced mathematical programming methods for supply chain management", presented by Andrey Kostin for the award of the degree of Doctor, has been carried out under our supervision at the Department of Chemical Engineering of the University Rovira i Virgili

Tarragona, 20th December, 2012

Dr. Gonzalo Guillén Gosálbez | Dr. Laureano Jiménez Esteller

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SUMMARY

The aim of this thesis is to provide a decision-support tool for the strategic planning of supply chains (SCs) considering several objectives simultaneously while taking also into account demand uncertainty. The general problem we aim to solve consists of determining the number, location and capacities of the SC facilities to be set up in each sub-region of a given country, their expansion policy over the planning horizon, the transportation requirements, and the production rates and flows of the involved feedstocks, wastes, and final products. To illustrate the capabilities of our approach, we use as a test-bed problem the design of supply chains for sugar and ethanol production in Argentina.

Particularly, in this thesis we present several modeling and decomposition strategies to solve the problem stated above. We first start by formulating a mixed-integer linear programming (MILP) model based on the Argentinean sugar cane industry. To encompass all possible conversion pathways, the proposed model includes production facilities of two types: sugar mills and distilleries. Depending on the utilized technology, the sugar mills can produce two main by-products: molasses or honey, both of which can be fermented to obtain bioethanol. The liquid and solid materials require different storage conditions, so the model considers two types of warehouses. The region of interest (i.e., Argentina) is subdivided into a number of sub-regions where the SC facilities can be installed. Different types of trucks are also considered for transporting materials between these sub-regions of the country. Numerical results produced with our MILP demonstrate that the centralized network is the preferred choice. Moreover, the production facilities should be located close to the sugar cane plantations. Among the technologies that convert sugar cane to white and raw sugars, the one producing honey as byproduct leads to better performance. We conclude also that ethanol should be produced by fermentation of either sugar cane juice or honey in sugar mills.

The complexity of this MILP model is mainly given by the number of integer and binary variables, both of which grow with the number of time intervals and sub-

regions. We found that large-scale problems with long-range planning horizons typically lead to intractable models. Hence, in order to reduce the computational burden of the MILP model, we propose a decomposition strategy (see [1] in Subsection 9.1). This technique is based on a "rolling horizon" scheme that decomposes the original problem into a number of smaller sub-problems that are solved in a sequential manner. The sub-problems of the decomposition algorithm are constructed by relaxing the integer variables denoting the number of transportation units, storages, and production facilities established in time periods beyond the first one. In each iteration, the method concentrates on determining the values of the integer variables corresponding to a single period, whereas the relaxed part of the problem allows assessing, in an approximate manner, the effect that these decisions have on later periods. Numerical examples show that the "rolling horizon" algorithm provides near optimal solutions(optimality gap lower than 3%) in a fraction of the time spent by CPLEX 12 [2].

After devising an efficient decomposition method for the MILP, we next studied the effects of demand uncertainty on the optimal strategic planning of sugarcane supply chains. To this end, we developed a two-stage stochastic MILP that maximizes the expected performance considering several financial risk mitigation options(see [3] in Subsection 9.2).

The last part of the thesis focuses on the optimization of sugarcane supply chains with economic and environmental concerns. Biofuels such as bioethanol are usually regarded as carbon neutral fuels, as they lead to zero overall CO2 emissions. Because of this, they can help mitigate global warming. Unfortunately, there are also some oft-overlooked aspects of biofuels, namely their potential impact on soils and groundwaters, that make them less appealing from an environmental standpoint. To properly assess the environmental benefits of biofuels, we need to consider the entire biofuel production chain. Furthermore, the environmental performance of biofuels can be further improved by optimizing their production-distribution supply chains according to economic and environmental concerns. This is the main goal of the emerging area known as Green Supply Chain Management (GrSCM) [4], which integrates environmental criteria within supply chain management.

Particularly, in this thesis we follow a combined approach that integrates mathematical programming with LCA [5] in order to optimize sugarcane supply chains considering simultaneously economic and environmental concerns. To explicitly incorporate the trade-off between economic and environmental issues, we formulated a bi-criterion MILP that seeks to optimize the net present value (NPV) and the environmental impact (measured through either the global warming potential, GWP100, or the Eco-indicator 99, EI99) (see [6] in Subsection 9.3). The resulting MILP problem was solved by use of the ε-constraint method. The Pareto-optimal solutions provided valuable insight into the design problem, and suggested process alternatives leading to environmental improvements. Additionally, we found that there is a clear trade-off between economic and environmental metrics, and also between the two environmental indicators optimized (i.e., EI99 and GWP100). This issue was further explored in the last part of the thesis.

Several authors have pointed out the existence of conflicts between environmental indicators in the optimization of biofuels facilities [7, 8]. Because of these inherent trade-offs, we may encounter solutions in which one environmental impact is reduced at the expense of increasing other negative effects. To avoid this situation, we need to apply holistic optimization methods that cover a wide variety of environmental impacts occurring throughout the entire production chain. Unfortunately, minimizing several environmental objectives simultaneously leads to hard optimization problems. While it is possible to merge single environmental objectives into aggregated indicators, this has the disadvantage of modifying the original dominance structure of the problem in a manner such that some optimal solutions might be left out of the analysis.

Bearing in mind all this, we developed in the last part of the thesis a rigorous computational framework for solving complex multi-objective optimization (MOO) problems that seek to optimize a large number of objectives simultaneously (see [9] in Subsection 9.4 and [10] in Subsection 9.5). The strategy proposed combines the traditional ε-constraint method [11] with an objective reduction algorithm. The latter allows identifying redundant objectives that can be omitted while still preserving the original dominance structure of the model, thereby reducing the associated computational complexity. By applying our rigorous approach, we found that several environmental effects of sugarcane SCs tend to be highly correlated, making it possible to perform the optimization in the space of a reduced set of key damages. Our approach facilitates the calculation and analysis of the Pareto-optimal solutions, providing valuable insight into the trade-offs arising between economic and environmental objectives, and ultimately guiding decision-makers towards the adoption of more sustainable alternatives.

Finally, it is worthy noting that the general approach and tools presented in this thesis can be applied to a wide variety of chemical (or related) processes[12].

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1 INTRODUCTION

The need for reducing the consumption of fossil fuels and associated environmental impact is driving the development of alternative "green" systems for energy production. One of the most successful examples of such shift is bioethanol, a fuel that has already proved its potential for replacing oil-based fuels in Brazil and the US [13]. Despite the effort made so far in the transition process towards a new energy system based on biofuels, there are still some important industrial aspects that merit further attention. In particular, one of the key points that still remains open is how to determine the optimal configuration of the production-distribution network capable of fulfilling a given ethanol demand in the growing markets. This is not a trivial task, since it requires the understanding of the complex temporal and spatial interdependencies arising between the SC entities.

In this thesis, we have developed several advanced mathematical strategies for the optimal design and planning of bioethanol SCs. These tools, which aim to facilitate decision-making in this area, include some novel features. First, they optimize environmental metrics in addition to the economic performance. Second, they account for demand uncertainty. Third, they expedite the search for optimal solution by use of decomposition algorithms that exploit the problem structure.

1.1 GENERAL OBJECTIVES

The objectives of this thesis are:

- Develop a systematic framework for the single objective (i.e. economic criterion) optimization of bioethanol SCs when all parameters are known in advance.
- Develop an algorithm to expedite the search for optimal solutions.
- Extend this framework so as to account for demand uncertainty.
- Develop a multi-objective optimization (MOO) framework for the environmentally conscious design and planning of SCs.

- Develop effective dimensionality reduction methods for facilitating the solution of MOO problems with a large number of objectives.

1.2 Problem statement

The MILP model of bioethanol SCs has to determine the structure of a three-echelon SC (production-storage-market). This network includes a set of production and storage facilities that can be installed in a set of disperse sub-regions. As mentioned, three types of models (deterministic, stochastic, and multi-objective) are developed. The deterministic problem can be formally stated as follows:

Given are a fixed time horizon, a set of product prices and demands, cost parameters for production , storage and transportation of materials, minimum and maximum capacity of plants, storages and transportation links, capital cost data, interest rate, landfill tax and upper limit for capital investment.

The goal is to determine the configuration of the bioethanol network and the associated planning decisions with the goal of maximizing the NPV. The model determines the number, location, capacity of production plants and warehouses to be set up in each grid, their capacity expansion policy, the transportation links and transportation modes that need to be established in the network, the production rates and flows of feed stocks, wastes and final products, as well as the prices of final products and demands over the planning horizon.

In the case of the stochastic model, we assume that the demand can be not perfectly known in advance (i.e., unknown demand), but can be described using scenarios with known probability of occurrence. Thus, the goal of the stochastic model is to maximize the expected NPV.

The multi-objective model optimizes a set of environmental indicators in addition to the profit. These environmental indicators are based on LCA principles.

The thesis report is organized as follows. The section that follows briefly outlines the mathematical programming tools developed in this research. The focus then turns to the assessment of the environmental damages of sugarcane SCs using different methodologies. Section 5 describes the application of the aforementioned optimization and assessment methods to the optimal design and planning of bioethanol SCs.

Finally, the conclusions of the work are drawn and future research lines that could extend and improve the framework proposed herein are outlined.

2 Application of mathematical programming to the bioethanol industry

The reader is referred here to the introduction sections of the papers of the thesis. Mathematical programming tools used in the optimization of bioethanol SCs are reviewed [1] (see Subsection 9.1). Most of these models deal only with tactical decisions and assume an existing network topology. Stochastic formulations are reviewed in Subsection 9.2. These models tend to optimize the expected performance and neglect financial risk management. Finally, multi-objective models are reviewed in [3] (see Subsection 9.2). Finally, the overview of the multi-objective models is presented in [9] (see Subsection 9.3). Most of these models are bi-objective, and none of them consider more than one environmental metric. Our works ([9] in Subsection 9.4 and [10] in Subsection 9.5) aim to fill this gap. We next describe briefly the mathematical tools used in this thesis.

3 Mathematical programming

Mathematical programming deals with the problem of maximizing or minimizing an objective function in the presence of constraints which are either inequalities ($g_n(x)$) or equalities ($h_{n'}(x)$). Consider the following single-objective (SO) minimization problem:

$$SO(X) = \min_{x \in X}(f(x))$$

subject to

$$g_n(x) \leq 0, \quad n = 1, 2, \ldots, N \tag{1}$$

$$h_{n'}(x) = 0, \quad n' = 1, 2, \ldots, N'$$

where $f(x)$ is an objective function. N is the number of inequality constraints, and N' is the number of equality constraints. X is the search space, and x is a vector of decision variables. If the objective function and the constraints are all linear, it is a linear programming (LP) problem. The problem takes the form of a nonlinear programming (NLP) model if at least one of the functions defining the objective function or the constraints is nonlinear. LP and NLP problems require in general different solution algorithms. If an LP problem contains discrete variables (integer or logical) in addition to continuous ones, then it becomes a mixed-integer linear programming (MILP) problem. Mixed-integer nonlinear programming (MINLP) problems contain at least one nonlinear equation. All of the models developed in this thesis are MILPs.

3.1 Methods for solving MILP problems

The MILP models were written and solved in the General Algebraic Modeling System (GAMS) [14]. GAMS is a high level modeling system for mathematical programming and optimization. It consists of an integrated development environment (IDE) connected to a group of optimization solvers. IDE allows the user to express optimization models in the special programming language called Algebraic Modeling Languages (AML) and then call appropriate solver to obtain a solution. Particularly, ILOG CPLEX [2] solver was used to solve the MILP problems in this work. CPLEX is known as the one of the most efficient algorithm for solving this type of problems.

To help computations and improve the numerical performance of CPLEX, we propose a rolling horizon strategy. The key idea of this strategy is to exploit the tight relaxation that is obtained when some of the integer variables of the problem are relaxed. Hence, the algorithm solves a sequence of MILPs, one for each time period, in which some of the discrete variables of the time periods beyond the ones being solved are relaxed. The integer solutions obtained in each run of the model are fixed for the corresponding time period being solved, and the problem is then resolved for subsequent intervals until all the integer variables are calculated. Further details of this algorithm can be found in [1] (see Subsection 9.1).

3.2 Optimization under uncertainty

Next, we switched to the problem of the strategic planning of SCs under uncertainty in the product demand. A two-stage stochastic model is derived in which the network design decisions, namely locations, capacities and number of plants and storage facilities, are regarded as first-stage variables. On the other hand, the production rates, the flows of materials between the SC entities and the product are considered as second-stage decision variables that must be taken once the uncertainty (i.e., the demand) is unveiled.

To incorporate the trade-off between expected profit and risk that naturally exists in an uncertain environmental of this type, we employ the SAA algorithm [15]. This method is based on generating a set of solutions, each of which showing a different behavior in the face of uncertainty. These solutions, which are obtained by solving the problem for each possible materialization of the uncertain parameters (i.e., for each scenario), are filtered according to some risk metrics in order to allow discarding those that show poor performance. The detailed explanation of this method is presented in [3] (see Subsection 9.2)

3.3 Multi-objective optimization

The MOO problem, MO(X), can be presented as follows:

$$MO(X) = \min_{x \in X} (F(x) = \{f_1(x), \dots, f_k(x), \dots, f_O(x)\})$$

subject to

$$g_n(x) \leq 0, \quad n = 1, 2, \dots, N \tag{2}$$
$$h_{n'}(x) = 0, \quad n' = 1, 2, \dots, N'$$

where O objective functions are optimized. $F(x)$ denotes the vector of objective functions $f_k(x)$. The set of values taken by the objective functions $f_k(x)$ in the feasible solutions of MO(X) constitutes the feasible objective space Z. In the context of our problem, one of the objectives f_k represents the economic performance (NPV), whereas the others quantify a set of environmental impacts. In [9] (see Subsection 9.4), the concepts of dominance and Pareto optimality are presented. The Pareto-optimal solutions in this work are obtained by means of the ε-constraint method [11].

3.3.1 ε-CONSTRAINT METHOD

The ε-constraint method entails solving a set of single objective problems $SO_e(X)$ where one objective is kept in the objective function (e.g., f_1) while the rest are transferred to auxiliary constraints in which upper bounds are imposed on them using a set of ε-parameters:

$$\begin{aligned} SO_e(X) = & \min_{x \in X}(f_1(x)) \\ \text{subject to } & g_n(x) \leq 0, \quad n = 1,2,\ldots,N \\ & h_{n'}(x) = 0, \quad n' = 1,2,\ldots,N' \\ & f_k(x) \leq \varepsilon_{k,e} \quad k = 2,\ldots,O \\ & \underline{\varepsilon_k} \leq \varepsilon_{k,e} \leq \overline{\varepsilon_k} \quad k = 2,\ldots,O \end{aligned} \tag{3}$$

Different Pareto solutions can be obtained by solving iteratively problem $SO_e(X)$ for different values of $\varepsilon_{k,e}$. We retain the NPV ($k = 1$) as main objective and transfer the environmental indicators ($k \neq 1$) to the auxiliary constraints. The lower and upper limits of each ε-parameter are obtained from the minimization of each separate environmental objective:

$$\begin{aligned} \underline{s_k} = & \arg\min_{x \in X}(f_k(x)), \ k \neq 1 \\ \text{subject to } & g_n(x) \leq 0, \quad n = 1,2,\ldots,N \\ & h_{n'}(x) = 0, \quad n' = 1,2,\ldots,N' \end{aligned} \tag{4}$$

which defines $\underline{\varepsilon_k} = f_k(\underline{s_k}), k \neq 1$. The maximum values of every objective f_k among the solutions $\underline{s_k}$ were used as the upper bounds for ε-parameters.

Next, the intervals $[\underline{\varepsilon_k}, \overline{\varepsilon_k}]$ are subdivided into —E_k— sub-intervals, and model

$SO_e(X)$ is solved for each of the limits of these sub-intervals, generating a different Pareto solution in each run. The detailed explanation of the algorithm can be found in [16].

3.3.2 Redundancy in MOO problems

In the context of MOO, several objective functions may exhibit a conflict with the remaining ones, whereas it is possible that some of objectives do not conflict. The non-conflicting objectives are regarded as redundant or non-essential. They can be removed from the MOO problem without changing the dominance structure. The concept of redundant objectives and a measure of changing original dominance structure are presented in [9] (see Subsection 9.4) and in [10] (see Subsection 9.5).

3.3.3 Objective reduction methods

In this thesis, the method originally proposed by [17] is utilized to find the set of redundant objectives. The explanation of the method is given in [9] (see Subsection 9.4) and in [10] (see Subsection 9.5).

4 Environmental assessment methods

In this thesis, the assessment of the environmental damages was conducted according LCA methodologies. Particularly, the environmental performance was measured by GWP100, EI99, damage to human health (DHH), damage to ecosystems quality (DEQ), and depletion of resources (DR). The computing of these metrics followed the LCA procedures [18]: goal and scope definition, inventory analysis, damage assessment and interpretation. The details of these stages are described in [6] (see Subsection 9.3).

5 Case study: Argentinean bioethanol industry

The mathematical model presented in this study is adopted to the sugarcane industry of Argentina. The formulation, however, is general enough to be easily extended to any other supply chains with similar characteristics. The details of the case-study can be found in [3] (see Subsection 9.1).

5.1 Production facilities

We assumed that the juice is extracted from sugarcane mainly by milling. Sugar mills use this juice to produce white sugar and raw sugar. There are two technologies that follow the "sugarcane-to-sugar" pathway. One of them generates molasses (T1) as a byproduct, whereas the other one produces a secondary honey (T2) in addition to sugars. These two byproducts differ in their sucrose content. Molasses is a viscous dark honey whose low sucrose content cannot be separated by crystallization, while the secondary honey is a honey with a larger amount of sucrose that leaves the sugar mill before being exhausted by crystallization. Anhydrous ethanol can be produced by fermentation and subsequent dehydration of different process streams: molasses (T3), honey (T4), and sugarcane juice (T5). Thus, the model considers a total of five different technologies, two for sugar production and three types of distilleries. The details of each technology, including the mass balance, are shown in Figure 2 from [3] (see Subsection 9.2), where residuals, loses and discards are omitted.

5.2 Storages

The model includes two different types of warehouses: storages for liquid products (S1), and storages for solid materials (S2). For each storage facility type, we consider specific fixed capital and unit storage costs, along with lower and upper limits on its capacity expansions. Similarly, as with the plants, the storage capacity might be expanded in order to follow changes in the demand as well as in the supply.

5.3 Transportation units

Transportation units deliver the final products to the customers, supply the production plants with raw materials, and dispose the process wastes. The model assumes that the materials can be transported by three different types of trucks: heavy trucks with open-box bed for sugar cane (TR1), medium trucks for sugar (TR2), and tank trucks for liquid products (TR3). Each transportation mode has fixed capital and unit transportation costs, and lower and upper limits on its capacity. Both storage and transportation modes considered in the model are shown in Figure 3 from [3] (see Subsection 9.2).

5.4 Region of interest: Argentina

The problem consists of 24 sub-regions representing the Argentinean provinces with corresponding demand of sugar and ethanol. Distances between sub-regions were determined considering the capitals of the provinces. We assumed that each sub-region has an associated sugar cane capacity. Particularly, sugar cane plantations are situated in five Argentinean provinces (see Figure 14 [1] in Subsection 9.1). The remaining sub-regions have to import sugar cane from these provinces. The economical parameters can be found in [1] in Subsection 9.1, whereas environmental ones are described in [6] in Subsection 9.3.

5.5 MILP models

The MILP models include three main blocks of equations: mass balances, capacity constraints and objective function/s. The equations of the deterministic version are explained in [1] (see Subsection 9.1) whereas the stochastic variant is given in [3] (see Subsection 9.2) The equations describing the environmental metrics can be found in [6], (see Subsection 9.3). The MILP model for computing the error of omitting objectives is presented in [10] in Subsection 9.5.

6 Conclusions

The methods developed in this thesis work provided a set of conclusions listed below:

- Three types of mathematical models (deterministic, stochastic, and multi-objective) for optimal design and planning of bioethanol SCs were developed and applied to the case study of the sugarcane industry in Argentina.

- Decomposition algorithm based on relaxation integer variables was implemented to overcome computational difficulties of solving large MILP problems. Numerical experiments showed that the decomposition algorithm is able to provide near optimal solutions in a fraction of time spent by CPLEX 12.

- The two stage stochastic model considering uncertainty in both ethanol and sugar demands was solved applying SAA algorithm. A set of SC configurations that behave in different ways in the face of uncertainty was obtained as the output of SAA. The analysis of the stochastic results revealed that there are two critical factors that influence the SC performance: production capacity and the number of storages and transportation units. Risk-taker strategies imply production facilities with larger capacities. Risk-averse SC configurations use more trucks and warehouses as compared to the rick-taker ones. It allows risk-averse SC configurations to be more flexible, however, it requires larger capital investments.

- Two bi-criteria models "NPV vs. GWP100" and "NPV vs. EI99" were solved via the ε-constraint method. The Pareto-optimal solutions demonstrated how significant environmental savings can be attained by properly adjusting SC operating conditions and topology. Moreover, the conflict between GWP100 and EI99 metrics was revealed.

- The rigorous MILP-based dimensionality reduction method was used to discover the possible conflicts between environmental metrics and to find the redundant objectives which can be omitted from the MOO problem. The results demonstrated that EI99, DHH, and DEQ behave in a similar manner. This makes possible to perform optimization problems with the reduced set of objectives and therefore to facilitate the solving procedure. The relationships between the retained environmental metrics have been investigated and the sources of the conflicts have been discovered.

- The method integrating the aforementioned rigorous MILP-based dimensionality reduction technique with the classical ε-constraint algorithm was applied. The results demonstrated that this combination leads to significant savings in time, producing Pareto sets of higher quality in a fraction of the CPU time spent by the stand alone ε-constraint. Furthermore, the method facilitates also the post optimal analysis of the Pareto solutions and provides valuable insight into the relationships between the LCA metrics of concern for decision-makers.

7 Future work

A set of potential research lines related to the material presented in this thesis is presented below:

- We would like to include the second generation technologies for ethanol production. These technologies allow converting woody biomass or forestry wastes to bioethanol [19]. The set of transportation technologies could be extended by adding the possibilities of transporting bioethanol via railroads, river barges, cabotage, and alcoholductes [20]. The possible environmental benefits of the new technologies could be investigated following the proposed holistic approach.

- Other biofuels, their production technologies, and possible feedstocks could be included in the framework and investigated. This may highlight the best bio-based alternatives of fossil fuels suited for the Argentinean economy.

- The scope of the study can be switched from Argentina to Brazil or the US where capacity of bioethanol production is higher. Hence, optimization of bioethanol the SCs may propose larger economical and environmental savings.

- The uncertainty not only in the product demands but also in the prices and environmental impacts can be investigated by applying the stochastic programming tools.

- Random generation (uniform random numbers, Sobol and Halton sequences) of the ε-bounds can be investigated. These methods can be compared in terms of the number of feasible iterations, unique solutions, CPU time, and the quality of the Pareto sets obtained

- We would like to apply the tools developed herein to other chemicals SCs: petrochemicals, detergents, hydrogen, etc.

8 NOMENCLATURE

Abbreviations

DEQ	damage to ecosystems quality
DHH	damage to human health
DR	depletion of resources
EI99	eco-indicator 99
GAMS	general algebraic modeling system
GrSCM	green supply chain management
GWP100	global warming potential over a 100-year time horizon
IDE	integrated development environment
LCA	life cycle assessment
LP	linear programming
NLP	nonlinear programming
MILP	mixed-integer linear programming
MINLP	mixed-integer nonlinear programming
NPV	net present value
SAA	sample average approximation
SC	supply chain
SCM	supply chain management

Indices

e	epsilon iterations
k	objectives
n	inequality constraints
n′	equality constraints

Sets

F	set of objectives
g	set of inequality constraints
h	set of equality constraints

Parameters

N	number of inequality constraints
N′	number of equality constraints
O	number of objectives

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9 RESEARCH ARTICLES

The results of this research were published in five journal articles, which are presented below.

9.1 A novel rolling horizon strategy for the strategic planning of supply chains. Application to the sugar cane industry of Argentina

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A novel rolling horizon strategy for the strategic planning of supply chains. Application to the sugar cane industry of Argentina

A.M. Kostin[a], G. Guillén-Gosálbez[a,*], F.D. Mele[b], M.J. Bagajewicz[c], L. Jiménez[a]

[a] Departament d'Enginyeria Química (EQ), Escola Tècnica Superior d'Enginyeria Química (ETSEQ), Universitat Rovira i Virgili (URV), Campus Sescelades, Avinguda Països Catalans 26, 43007 Tarragona, Spain
[b] Dpto. Ingeniería de Procesos, FACET, Universidad Nacional de Tucumán, Av. Independencia 1800, S.M. de Tucumán T4002BLR, Argentina
[c] School of Chemical, Biological and Materials Engineering, University of Oklahoma, Norman, OK 73019, USA

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ABSTRACT

In this article, we propose a new method to reduce the computational burden of strategic supply chain (SC) planning models that provide decision support for public policy makers. The method is based on a rolling horizon strategy where some of the integer variables in the mixed-integer programming model are treated as continuous. By comparing with rigorous solutions, we show that the strategy works efficiently. We illustrate the capabilities of the approach presented by its application to a SC design problem related to the sugar cane industry in Argentina. The case study involves determining the number and type of production and storage facilities to be built in each region of the country so that the ethanol and sugar demand is fulfilled and the economic performance is maximized.

1. Introduction

Supply chain management (SCM) has recently gained wider interest in both, academia and industry, given its potential to increase the benefits through an efficient coordination of the operations of supply, manufacturing and distribution carried out in a network (Naraharisetti, Adhitya, Karimi, & Srinivasan, 2009; Puigjaner & Guillén-Gosálbez, 2008). In the context of process systems engineering (PSE), these activities are the focus of the emerging area known as Enterprise Wide Optimization (EWO), which as opposed to SCM, places more emphasis on the manufacturing stage (Grossmann, 2005).

The SCM problem may be considered at different levels depending on the strategic, tactical, and operational variables involved in the decision-making process (Fox, Barbuceanu, & Teigen, 2000). The strategic level is based on those decisions that have a long-lasting effect on the firm. These include, among many others, the SC design problem, which addresses the optimal configuration of an entire SC network. The tactical level encompasses long- to medium-term management decisions, which are typically updated a few times every year, and include overall purchasing and production decisions, inventory policies, and transport strategies. Finally, the operational level refers to day-to-day decisions such as scheduling, lead-time quotations, routing, and lorry loading (Guillén-Gosálbez, Espuña, & Puigjaner, 2006).

In the recent past the SCM tools developed in these hierarchical levels have primarily focused on maximizing the economic performance in the private sector. By contrast, the academic literature on SCM applications for public policy makers is still quite scarce (see Preuss, 2009). The use of SCM tools in the latter area is very promising, since they can provide valuable insight into how to satisfy the population's needs in an efficient manner, thus guiding government authorities towards the adoption of the best technological alternatives to be promoted and eventually established in a given country.

The goal of this paper is to provide a general modeling framework and a solution strategy for SC design problems, with focus on the strategic level of SCM, and with special emphasis on applications found in the public sector. Particularly, given a set of available production, storage and transportation technologies that can be adopted in different regions of a country, the goal of the analysis performed is to determine the optimal SC configuration, including the type of technologies selected, the capacity expansions over time, and their optimal location, along with the associated planning decisions that maximize a given economic criterion. In this work, such a design task is formulated in mathematical terms as a mixed-integer programming problem with a specific structure that includes integer and binary variables of different nature. To

* Corresponding author. +34 977 558 618; fax: +34 977 559 621.
E-mail addresses: andrey.kostin@urv.cat (A.M. Kostin), gonzalo.guillen@urv.cat (G. Guillén-Gosálbez), fmele@herrera.unt.edu.ar (F.D. Mele), bagajewicz@ou.edu (M.J. Bagajewicz), laureano.jimenez@urv.cat (L. Jiménez).

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Nomenclature

Indices

- i materials
- g sub-region zones
- l transportation modes
- p manufacturing technologies
- s storage technologies
- t time periods

Sets

- $IL(l)$ set of materials that can be transported via transportation mode l
- $IM(p)$ set of main products for each technology p
- $IS(s)$ set of materials that can be stored via storage technology s
- $LI(i)$ set of transportation modes l that can transport material i
- SEP set of products that can be sold
- $SI(i)$ set of storage technologies that can store materials i

Parameters

- α^{PL}_{pgt} fixed investment coefficient for technology p
- α^{S}_{sgt} fixed investment coefficient for storage technology s
- β storage period
- β^{PL}_{pgt} variable investment coefficient for technology p
- β^{S}_{sgt} variable investment coefficient for storage technology s
- ρ_{pi} material balance coefficient of material i in technology p
- τ minimum desired percentage of the available installed capacity
- φ tax rate
- avl_l availability of transportation mode l
- $CapCrop_{gt}$ total capacity of sugar cane plantations in sub-region g in time t
- DW_{lt} driver wage
- $EL_{gg'}$ distance between g and g'
- $\overline{FCI}$ upper limit for capital investment
- FE_l fuel consumption of transport mode l
- FP_{lt} fuel price
- GE_{lt} general expenses of transportation mode l
- LT_{ig} landfill tax
- ME_l maintenance expenses of transportation mode l
- $\overline{PCap_p}$ maximum capacity of technology p
- $\underline{PCap_p}$ minimum capacity of technology p
- PR_{igt} prices of final products
- $\overline{Q_l}$ maximum capacity of transportation mode l
- $\underline{Q_l}$ minimum capacity of transportation mode l
- $\overline{SCap_s}$ maximum capacity of technology p
- $\underline{SCap_s}$ minimum capacity of storage technology s
- SD_{igt} actual demand of product i in sub-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

- CF_t cash flow in time t
- DC_t disposal cost in time t
- DTS_{igt} delivered amount of material i in sub-region g in period t
- FC_t fuel cost
- FCI fixed capital investment
- FOC_t facility operating cost in time t
- $FTDC_t$ fraction of the total depreciable capital in time t
- GC_t general cost
- LC_t labor cost
- MC_t maintenance cost
- NE_t net earnings in time t
- NP_{pgt} number of installed plants with technology p in sub-region g in time t
- NPV net present value of SC
- NS_{sgt} number of installed storages with storage technology s in sub-region g in time t
- NT_{lt} number of transportation units l
- $PCap_{pgt}$ existing capacity of technology p in sub-region g in time t
- $PCapE_{pgt}$ expansion of the existing capacity of technology p in sub-region g in time t
- $Q_{ilgg't}$ flow rate of material i transported by mode l from sub-region g' to current sub-region g in time period t
- Rev_t revenue in time t
- RNP_{pgt} "relaxed" number of installed plants with technology p in sub-region g in time interval t
- RNS_{sgt} "relaxed" number of installed storages with storage technology s in sub-region g in time interval t
- RNT_{lt} "relaxed" number of transportation units l in time interval t
- $SCap_{sgt}$ capacity of storage s in sub-region g in time t
- $SCapE_{sgt}$ expansion of the existing capacity of storage s in sub-region g in time t
- ST_{isgt} total inventory of material i in sub-region g stored by technology s in time t
- TOC_t transport operating cost in time t
- PE_{ipgt} production rate of material i in technology p in sub-region g in time t
- PT_{igt} total production rate of material i in sub-region g in time t
- PU_{igt} purchase of material i in sub-region g in time t
- $X_{lgg't}$ binary variable, which is equal to 1 if material flow between two sub-regions g and g' is established and 0 otherwise
- W_{igt} amount of wastes i generated in sub-region g in period t

expedite the solution of such formulation, we propose a novel decomposition method based on a customized "rolling horizon" algorithm that achieves significant reductions in CPU time while still providing near optimal solutions.

The paper is organized as follows. First, a literature review on strategic SCM tools based on mathematical programming is presented, followed by a more specific review on the particular application of these techniques to the sugar cane industry. A formal definition of the problem under study is given next along with its mathematical formulation. The following section introduces a tailor-made decomposition strategy that reduces the computational burden of the model by exploiting its mathematical structure. The capabilities of the proposed modeling framework and solution strategy are illustrated next through a case study based on the sugar cane industry of Argentina. The conclusions of the work are finally drawn in the last section of the paper.

1.1. Mathematical programming approaches for strategic SCM problems

Optimization using mathematical programming is probably the most widely used approach in SCM. General literature reviews can be found in the work by Mula, Peidro, Díaz-Madroñero, and Vicens (2010), whereas a more specific work devoted to process industries can be found in the articles by Grossmann (2005) and Papageorgiou (2009). The preferred modeling tool for addressing strategic SCM problems has been mixed-integer linear programming (MILP). MILP models for SCM typically adopt fairly simple aggregated representations of capacity that avoid nonlinearities. This feature has been the key of their success, since it has allowed them to be easily adapted to a wide range of industrial applications. In these MILP formulations, continuous variables are used to represent materials flows and purchases and sales of products, whereas binary variables are employed to model tactical and/or strategic decisions associated with the network configuration, such as selection of technologies and establishment of facilities and transportation links (Guillén-Gosálbez, Mele, Espuña, & Puigjaner, 2006; Laínez, Guillén-Gosálbez, Badell, Espuña, & Puigjaner, 2007).

Several solution strategies have been explored for effectively solving these strategic SCM problems. Bok, Grossmann, and Park (2000) reported an implementation of a bi-level decomposition algorithm to solve a MILP model that maximized the profit of a network showing that this algorithm could reduce the solution time by half compared to the full space method implemented in CPLEX. Guillén-Gosálbez, Mele, and Grossmann (2010) presented also a bi-level algorithm for solving the strategic planning of hydrogen SCs for vehicle use. Using numerical examples, they showed that the decomposition method could achieve a reduction of one order of magnitude in CPU time compared to the full space method (the whole model without decomposition, relaxation or approximations) while still providing near optimal solutions (i.e., with less than 1% of optimality gap).

Lagrangean decomposition has also been used in strategic SCM problems. Gupta and Maranas (1999) applied Lagrangean decomposition to solve a planning problem that considered different products and manufacturing sites. With this decomposition technique, the authors obtained a solution with an optimality gap of 1.6%, reducing in one order of magnitude the CPU time required by CPLEX 4.0 to find a solution with a gap of 3.2%. You and Grossmann (2010) introduced a spatial decomposition algorithm based on the integration of Lagrangean relaxation and piecewise linear approximation to reduce the computational expense of solving multi-echelon supply chain design problems in the presence of uncertain customer demands. Chen and Pinto (2008) investigated the application of various Lagrangean-based techniques including Lagrangean decomposition, Lagrangean relaxation, and Lagrangean/surrogate relaxation, coupled with subgradient and modified subgradient optimization. The comparison showed that the proposed strategies are much more efficient than the full space method. Particularly, they concluded that the computational time was greatly reduced while still achieving optimality gaps of less than 2%.

Other solution methods applied to SCM problems have been Bender's decomposition (Geoffrion & Graves, 1974) and "rolling horizon" algorithms based on the original work by Wilkinson (1996). The former approach has been mainly used in the context of strategic/tactical SCM problems (Cordeau, Pasin, & Solomon, 2006; Dogan & Goetschalckx, 1999; MirHassani, Lucas, Mitra, Messina, & Poojari, 2000; Paquet, Martel, & Desaulniers, 2004; Santoso, Ahmed, Goetschalckx, & Shapiro, 2005; Uster, Easwaran, Akcali, & Cetinkaya, 2007), whereas the latter strategy has been typically applied to operational SCM problems (Dimitriadis, Shah, & Pantelides, 1997; Elkamel & Mohindra, 1999; Balasubramanian & Grossmann, 2004). Rolling horizon algorithms are based on approximating the solution of the full space model by a set of sub-models, each of which representing only part of the planning horizon in detail. This strategy has been shown to be very efficient in solving scheduling problems with large time horizons (Van den Heever & Grossmann, 2003). However, to our knowledge, it has never been applied to strategic SCM problems.

1.2. Applications of mathematical programming to the sugar cane industry

The interest in renewable fuels such as bioethanol and other bio-fuels has greatly increased in the last years all over the world. Following this trend, Argentina approved the National Act 26,093, which aims to promote the production of bioethanol for fuel blending. This new legislation represents a major challenge for the sugar cane industry, which must increase its flexibility and efficiency in order to satisfy the growing sugar and bioethanol demand. The final goal of this law is to promote the adoption of proper energetic and environmental policies.

The interest on ethanol has motivated the development of mathematical programming tools for optimizing its production. The models presented so far have mainly focused on studying the individual components of the ethanol SC rather than optimizing all its entities in an integrated manner. Particularly, Yoshizaki, Muscat, and Biazzi (1996) introduced a LP model to find the optimal distribution of sugar cane mills, fuel bases and consumer sites in southeastern Brazil. Kawamura, Ronconi, and Yoshizaki (2006) presented a LP model to minimize the transportation and external storage costs of the existing SC in Brazil. Ioannou (2005) applied a LP optimization model to reduce the transportation cost in the Greek sugar industry, while Milán, Fernández, and Pla Aragonés (2006) introduced a MILP model to minimize the transportation cost of a sugar cane SC in Cuba. Dunnett, Adjiman, and Shah (2008) developed a combined production and logistic model to find the optimal configuration of a lignocellulosic bioethanol SC. Mathematical programming methods associated with plantation planning and scheduling can be found in the works by Grunow, Guenther, and Westinner (2007), Paiva and Morabito (2009); Colin (2009) and Higgins and Laredo (2006).

As observed, most of the aforementioned approaches have focused on the tactical level of the SCM problem covering short/medium-term decisions associated with the SC operation. These methods consider a given SC configuration and attempt to optimize its activities without modifying the existing topology. A general modeling and solution framework for holistically optimizing ethanol infrastructures is currently lacking. Such an approach would enable governments to choose, in advance, the optimum configurations for ethanol production, storage and delivery systems. A systematic tool of this type could play a major role in guiding national and international policy makers towards the best decisions in the transition process from traditional fossil fuels to biofuels. In this article, we fill this research gap by proposing a novel mathematical formulation for the strategic planning of sugar cane SCs along with an efficient solution method that allows to tackle problems of realistic size in moderate CPU times.

2. Problem statement

To formally state the SC design problem, we consider a generic three-echelon SC (production–storage–market) like the

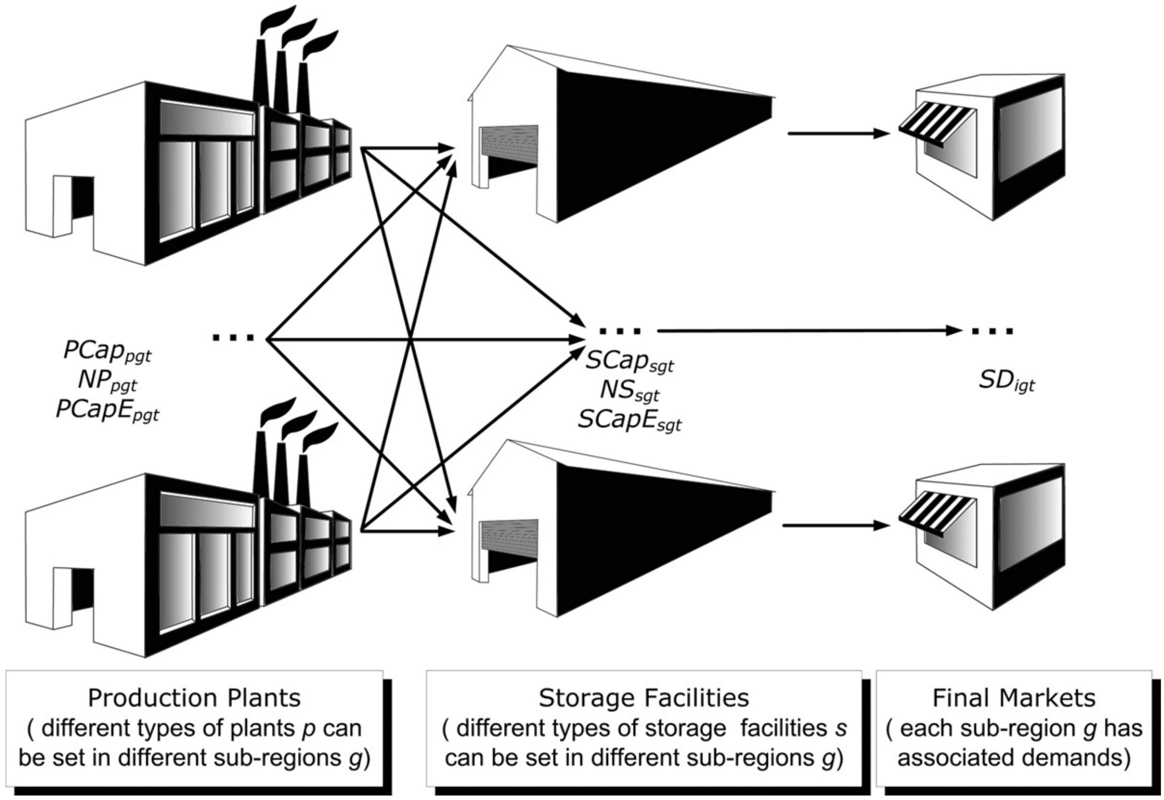

Fig. 1. Structure of the three-echelon ethanol/sugar SC.

one depicted in Fig. 1. This network includes a set of production and storage facilities, and final markets. We assume that we are given a specific region of interest that is divided into a set of sub-regions in which the facilities of the SC can be established in order to cover a given demand. In general, these sub-regions, which are regarded as potential locations for the SC entities, will be defined according to the administrative division of a country. The 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, tax rate, capacity data for plants, storages and transportation links, fixed capital investment data, interest rate, storage holding period and landfill tax. The goal is to determine the configuration of a three-echelon bioethanol network and associated planning decisions with the goal of maximizing the economic performance for a given time horizon. Decisions to be made include the number, location and capacity of production plants and warehouses to be set up in each sub-region, their capacity expansion policy for a given forecast of prices and demand over the planning horizon, the transportation links and transportation modes of the network, and the production rates and flows of feed stocks, wastes and final products.

3. Mathematical model

In this section, we present a mathematical model that considers the specific features of the sugar cane industry, while still being general enough to be easily adapted to any other industrial SC. Particularly, our model is based on the MILP formulation introduced by Almansoori and Shah (2006), and Guillén-Gosálbez et al. (2010), which addresses the design of hydrogen SCs. Furthermore, the model follows the SC formulation developed by Guillén-Gosálbez and Grossmann for the case of petrochemical SCs (Guillén-Gosálbez & Grossmann, 2009b; Guillén-Gosálbez & Grossmann, 2010a), in the way in which the mass balances are handled.

Compared to standard SC formulations that focus on the private sector, the model exhibits two main differentiating features. The first one is that plants, warehouses and final markets share the same potential locations. These locations correspond to the sub-regions in which the overall region of interest is divided. The second one is that the model accounts for the option of opening more than one facility in a given region and time period. This consideration requires the introduction of integer variables that increase the combinatorial complexity of the model. This structure is exploited by our solution algorithm.

As sugar and ethanol share the same feedstock, the proposed model includes integrated infrastructures for ethanol/sugar production. The mathematical formulation considers all possible configurations of the future ethanol/sugar SC as well as all technological aspects associated with the SC performance such as production and storage technologies, waste disposal, modes for transportation of raw materials, products and wastes. We describe next some general features of the model before immersion into a detailed description of its equations.

Production plants

Sugar cane is the leading feedstock for bioethanol production in Argentina as well as in most of the tropical regions all over the world (e.g., Brazil, India, China, etc.). The juice is extracted from sugar cane mainly by milling. From this step sugar cane juice can be treated in different ways. Sugar factories can use this juice to produce white sugar and raw sugar. There are two technologies realizing the "sugar cane-to-sugar" pathway: one of them generates molasses (T1) as a byproduct, whereas the other one provides a secondary honey (T2) in addition to sugars. These two kinds of byproducts are

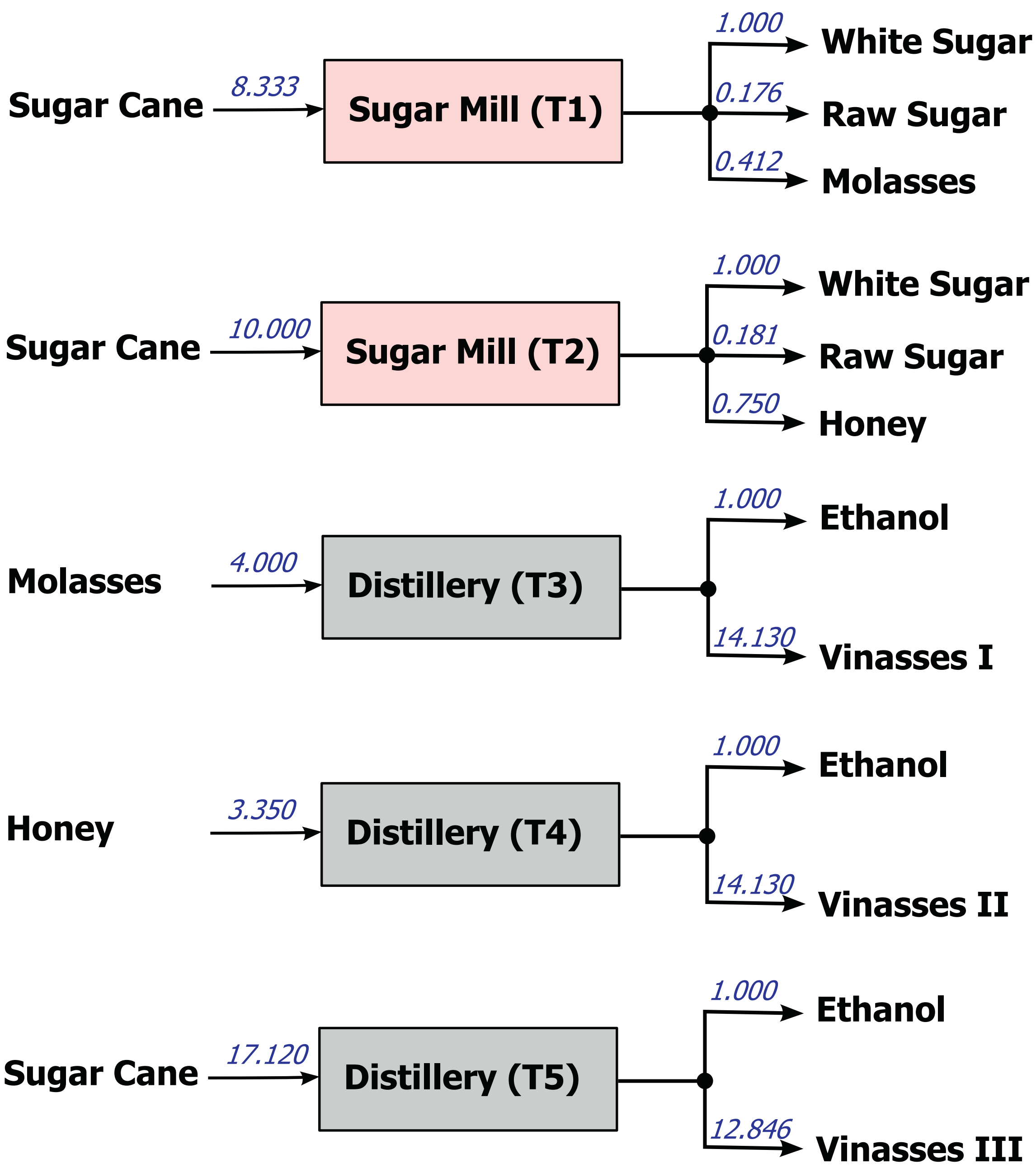

Fig. 2. Set of technologies. The labels T1, T2, . . ., T5 indicate the technology used; the numbers above the arrows correspond to the mass balance coefficients.

distinguished by their sucrose content. Molasses is a viscous dark honey whose low sucrose content cannot be separated by crystallization, while secondary honey is a honey with a larger amount of sucrose that leaves the sugar mill before being exhausted by crystallization. Anhydrous ethanol can be produced by fermentation and following dehydration of different process streams: molasses (T3), honey (T4) and sugar cane juice (T5). According to this, the model considers five different technologies, two for sugar production and three types of distilleries. The details of each technology, including the mass balance coefficients, are shown in Fig. 2. We assume that bagasse is completely utilized for internal purposes, 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.

All the considered technologies require a water feed. For example, sugar mills T1 and T2 use water for the imbibition of the chopped sugar cane. In the technologies T3 and T4, molasses or honey must be diluted before the fermentation step. Distillery T5 utilizes water for two purposes: extraction and dilution of sugar cane juice. We do not consider a water supply, but the cost of water is included in the parameter UPC_{ipgt} (unit production cost).

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 the sub-region, the capacity that the sub-region has to fulfill its internal needs and the cost data.

Storage facilities

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

We do not consider feed storage facilities in the supply chain. The reason for this is that the freshly cut sugar cane must be transported to the factory without any delay, because it loses its sugar content very rapidly. Moreover, damage to the cane during mechanical harvesting accelerates this decline. Hence, the sugar cane must be transported to a sugar mill within 24 hours after harvest at the latest (Shreve & Austin, 1984).

Transportation modes

Transportation links allow to deliver final products to customers, supply the 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 trucks with open-box bed for sugar cane, lorries for sugar and tank trucks for liquid products. Each type of transportation mode has fixed capital and unit transportation costs and lower and upper limits for its capacity. The number and capacity of the transportation links can also vary over time in order to follow a given demand pattern.

3.1. General constraints

We next describe the main mathematical constraints of the model, which have been derived bearing in mind the particular features of the sugar cane industry in Argentina.

Materials balance

The starting point for all design is the material balance. Particularly, the law of conservation of mass must be satisfied in every sub-region. The overall mass balance for each sub-region is represented by Eq. (1). In accordance with it, for every material form i, the initial inventory kept in sub-region g from 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 ($Q_{ilg'gt}$) must equal the final inventory (ST_{isgt}) plus the amount delivered to customers (DTS_{igt}) plus the output flow to other sub-regions ($Q_{ilgg't}$) and the amount of waste (W_{igt}).

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

In this equation, $SI(i)$ represents the set of technologies that can be used to store product i, whereas $LI(i)$ are the set of transportation modes that can transport product i. Furthermore, the amount of products delivered to the final markets should be less than or equal to the actual demand (SD_{igt}):

$$DTS_{igt} \le SD_{igt} \quad \forall i, g, t \tag{2}$$

Production

The total production rate of material i in sub-region g is determined from the particular production rates (PE_{ipgt}) of each technology p installed in the sub-region:

$$PT_{igt} = \sum_{p} PE_{ipgt} \quad \forall i, g, t \tag{3}$$

The details of each technology, including the mass balance coefficients, are shown in Fig. 2, where residuals, water feed, loses and discards are omitted. As observed, the material balance coefficients of the main products (white sugar and ethanol) have been normalized to 1. The production rates of byproducts and raw materials for each technology are calculated from the material balance coefficients, ρ_{pi}, and the production rates of the main products:

$$PE_{ipgt} = \rho_{pi} PE_{i'pgt} \quad \forall i, p, g, t, \ \forall i' \in IM(p) \tag{4}$$

In this equation, $IM(p)$ represents the set of main products associated with each technology. The values of the material balance coefficients are negative for feedstocks and positive for products/by-products. The production rate of each technology p in sub-region g is limited by the minimum desired percentage of the available technology that must be utilized, τ, multiplied by the existing capacity (represented by the continuous variable $PCap_{pgt}$) and the maximum capacity:

$$\tau PCap_{pgt} \le PE_{ipgt} \le PCap_{pgt} \quad \forall i, p, g, t \tag{5}$$

The capacity of technology p in any time period t is calculated adding the existing capacity at the end of the previous period to the expansion in capacity, $PCapE_{pgt}$, carried out in period t:

$$PCap_{pgt} = PCap_{pgt-1} + PCapE_{pgt} \quad \forall p, g, t \tag{6}$$

Eq. (7) bounds the capacity expansion $PCapE_{pgt}$ between upper and lower limits, which are calculated from the number of plants installed in the sub-region (NP_{gpt}) and the minimum and maximum capacities associated with each technology p ($\underline{PCap_p}$ and $\overline{PCap_p}$, respectively).

$$\underline{PCap_p} NP_{pgt} \le PCapE_{pgt} \le \overline{PCap_p} NP_{pgt} \quad \forall p, g, t \tag{7}$$

The purchases of sugar cane are limited by the capacity of the existing sugar cane plantation in sub-region g and time interval t:

$$PU_{igt} \le CapCrop_{gt} \quad \forall i = \text{sugar cane}, g, t \tag{8}$$

Storage

As occurs with plants, the storage capacity is limited by lower and upper bounds, which are given by the number of storage facilities installed in sub-region g (NS_{sgt}) and the minimum and maximum storage capacities ($\underline{SCap_s}$ and $\overline{SCap_s}$, respectively) associated with each storage technology:

$$\underline{SCap_s} NS_{sgt} \le SCapE_{sgt} \le \overline{SCap_s} NS_{sgt} \quad \forall s, g, t \tag{9}$$

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 ($SCapE_{sgt}$):

$$SCap_{sgt} = SCap_{sgt-1} + SCapE_{sgt} \quad \forall s, g, t \tag{10}$$

The storage capacity should be enough to store the total inventory (ST_{isgt}) of product i during time interval t:

$$\sum_{i \in IS(s)} ST_{isgt} \le SCap_{sgt} \quad \forall s, g, t \tag{11}$$

In this equation, $IS(s)$ denotes the set of products that can be stored by technology s. During steady-state operation, the average inventory (AIL_{igt}) is a function of the amount delivered to customers and the storage period β:

$$AIL_{igt} = \beta DTS_{igt} \quad \forall i, g, t \tag{12}$$

The storage capacity ($SCap_{sgt}$) that should be established in a sub-region in order to cope with fluctuations in both supply and demand, is twice the average inventory levels of products i (Simchi-Levi, Kamisky, & Simchi-Levi, 2000).

$$2AIL_{igt} \le \sum_{s \in SI(i)} SCap_{sgt} \quad \forall i, g, t \tag{13}$$

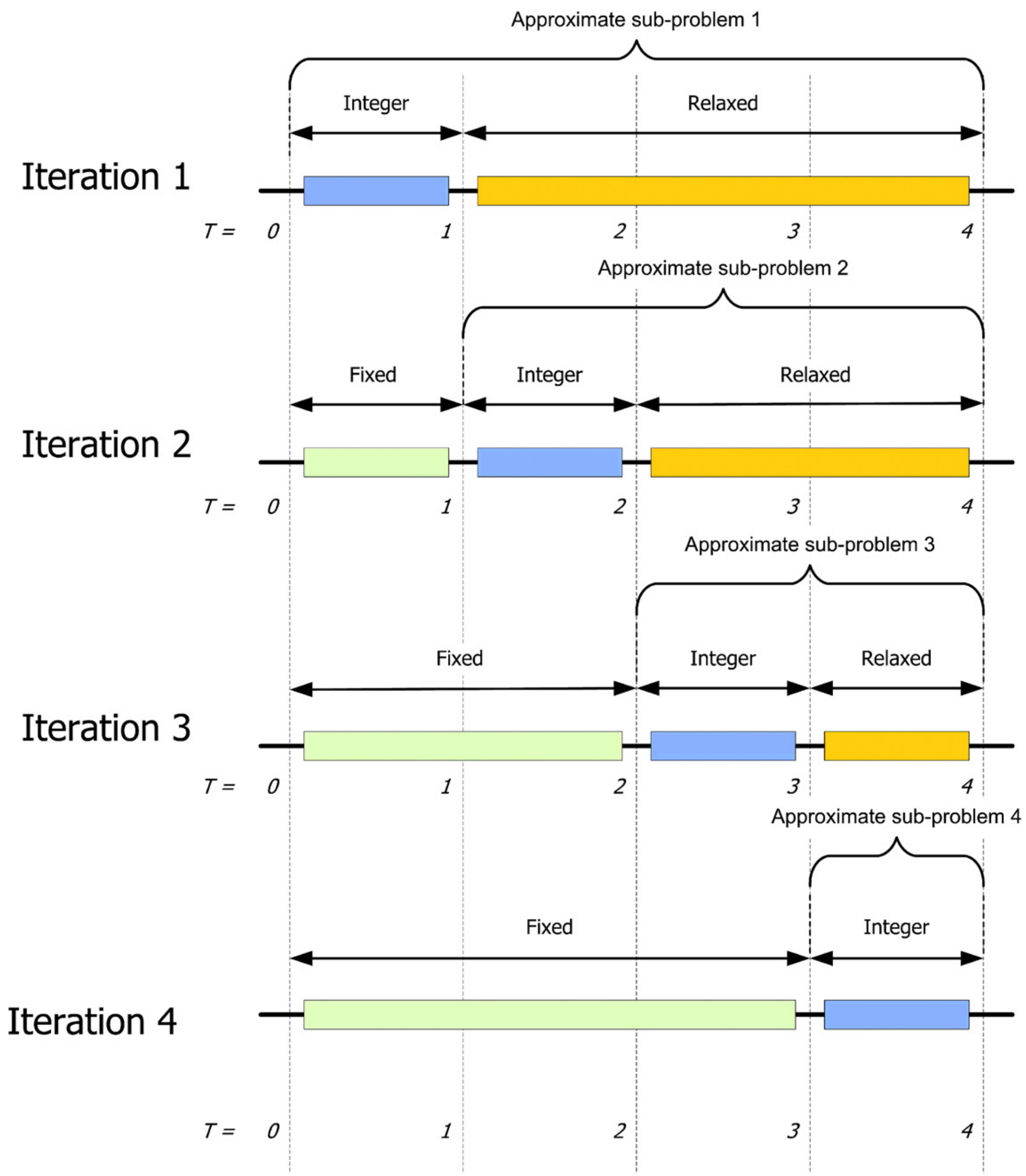

Fig. 3. Application of the "rolling horizon" strategy to a four-time-period problem.

Transportation

The existence of a transportation link between two sub-regions g and g' is represented by a binary variable $X_{lgg't}$ which equals 1 if a transportation link is established between the two sub-regions and 0 otherwise. The definition of this variable is enforced via Eq. (14), which constraints the materials flow between minimum and maximum allowable capacity limits ($\underline{Q_l}$ and $\overline{Q_l}$, respectively):

$$\underline{Q_l} X_{lgg't} \leq \sum_{i \in IL(l)} Q_{ilgg't} \leq \overline{Q_l} X_{lgg't} \quad \forall l, t, g, g'(g' \neq g) \tag{14}$$

In this equation, $IL(l)$ represents the set of materials that can be transported via transportation mode l. Furthermore, a sub-region can either import or export material i, but not both at the same time:

$$X_{lgg't} + X_{lg'gt} = 1 \quad \forall l, t, g, g'(g' \neq g) \tag{15}$$

3.2. Objective function

The use of *NPV* as an objective function is a widely-spread approach in investment planning. In most cases it results in a linear model, which can be effectively solved by standard branch-and-bound methods. However, the *NVP* measure does not account appropriately for the rate at which the investment is recovered because it tends to add investment that has marginal or meaningless returns. Bagajewicz (2008) pointed out that additional procedures and measures are needed in planning problems. Particularly, the return of investment (*ROI*) is a more appropriate key performance indicator when there are other investment alterna-

Table 1
Mean values for demand, ton/year.

Name of province	Associated sub-region	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	9714.57	4857.29	10,686.03
Mendoza	G06	43,565.35	21,782.67	47,921.88
Neuquén	G07	13,720.58	6860.29	15,092.64
Entre Rios	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	5758.64	12,669.00
Chaco	G11	26,439.66	13,219.83	29,083.63
Santa Cruz	G12	5708.56	2854.28	6279.42
Salta	G13	30,746.12	15,373.06	33,820.73
San Juan	G14	17,526.29	8763.14	19,278.92
San Luis	G15	11,016.52	5508.26	12,118.18
Tucumán	G16	37,155.73	18,577.87	40,871.31
Jujuy	G17	17,125.69	8562.84	18,838.26
Santa Fe	G18	81,121.68	40,560.84	89,233.85
La Pampa	G19	8412.62	4206.31	9253.88
Santiago del Estero	G20	21,732.60	10,866.30	23,905.86
Catamarca	G21	8612.92	4306.46	9474.21
Río Negro	G22	15,022.53	7511.27	16,524.79
Formosa	G23	13,520.28	6760.14	14,872.31
Tierra del Fuego	G24	3204.81	1602.40	3525.29

tives competing for the same capital. In the context of a SC design problem like the one addressed in this article, one way in which this metric can be evaluated is using the ratio between the average cash flows (CF_t) and the fixed capital investment FCI:

$$ROI = \frac{\left(\sum_t CF_t\right)/T}{FCI} \tag{16}$$

As observed, the introduction of the ROI as the economic indicator to be maximized gives rise to a mixed-integer linear fractional programming formulation that can be solved using the Dinkelbach's algorithm. Given that the linear NPV-based approach already has computational issues that this paper attempts to ameliorate, following Bagajewicz (2008) we resort to solving a series of MILPs that maximize the NPV for different upper bounds on FCI. As discussed in Bagajewicz (2008), from these results one can identify solutions close to the maximum ROI one.

The NPV can be determined from the discounted cash flows generated in each of the time intervals t in which the total time horizon is divided:

$$NPV = \sum_t \frac{CF_t}{(1+ir)^{t-1}} \tag{17}$$

In this equation, ir represents the interest rate. The cash flow that appears in Eq. (17) in each time period is computed from the net earnings NE_t (i.e., profit after taxes), and the fraction of the total depreciable capital ($FTDC_t$) that corresponds to that period as follows:

$$CF_t = NE_t - FTDC_t, \quad t = 1, \ldots, T-1 \tag{18}$$

In the calculation of the cash flow of the last time period ($t = T$), we assume that part of the total fixed capital investment 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.

$$CF_t = NE_t - FTDC_t + svFCI, \quad t = T \tag{19}$$

Table 2
Distances between sub-regions, 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	1167	1080	1178	511	1008	1379	953	2542	1542	1140	800	1229	1565	484	607	1070	1122	948	1098	3162
G02	711	0	900	768	460	680	1153	360	1118	1524	880	2638	844	600	420	597	867	340	667	439	433	1208	1031	3258
G03	933	900	0	990	1024	1490	1913	573	335	2206	20	3369	830	1460	1190	794	853	540	1388	635	857	1774	186	3989
G04	60	768	990	0	1224	1137	1159	568	1065	1371	1010	2533	1599	1197	857	1286	1622	541	664	1127	1173	924	1236	3153
G05	1167	460	1024	1224	0	612	1427	820	1333	1872	1007	3087	704	355	559	382	727	800	1015	389	171	1565	1139	3707
G06	1080	680	1490	1137	612	0	815	952	1710	1628	1470	2783	1311	166	264	872	1329	930	789	1007	725	1342	1600	3403
G07	1178	1153	1913	1159	1427	815	0	1413	2075	746	1880	1909	1997	981	890	1581	2020	1373	535	1618	1536	557	2020	2529
G08	511	360	573	568	820	952	1413	0	758	1715	590	2887	1107	950	691	794	1130	30	855	635	803	1252	746	3507
G09	1008	1118	335	1065	1333	1710	2075	758	0	2356	332	3511	1142	1708	1449	1086	1165	785	1518	927	1179	1896	508	4131
G10	1379	1524	2206	1371	1872	1628	746	1715	2356	0	2236	1172	2308	1705	1382	2107	2331	1685	857	1986	1900	809	2450	1792
G11	953	880	20	1010	1007	1470	1880	590	332	2236	0	3388	813	1460	1190	774	833	540	1368	618	820	1756	173	4008
G12	2542	2638	3369	2533	3087	2783	1909	2887	3511	1172	3388	0	3482	2868	2545	3192	3505	2850	2020	3070	3167	1952	3593	620
G13	1542	844	830	1599	704	1311	1997	1107	1142	2308	813	3482	0	1150	1264	310	90	1077	1462	472	533	2066	959	4102
G14	1140	600	1460	1197	355	166	981	950	1708	1705	1460	2868	1150	0	320	708	1163	920	848	840	497	1509	1540	3488
G15	800	420	1190	857	559	264	890	691	1449	1382	1190	2545	1264	320	0	838	1287	660	525	859	674	1087	1345	3165
G16	1229	597	794	1286	382	872	1581	794	1086	2107	774	3192	310	708	838	0	328	764	1257	164	221	1803	925	3812
G17	1565	867	853	1622	727	1329	2020	1130	1165	2331	833	3505	90	1163	1287	328	0	1092	1485	490	563	2095	921	4125
G18	484	340	540	541	800	930	1373	30	785	1685	540	2850	1077	920	660	764	1092	0	828	605	777	1218	709	3470
G19	607	667	1388	664	1015	789	535	855	1518	857	1368	2020	1462	848	525	1257	1485	828	0	1129	1065	580	1492	2640
G20	1070	439	635	1127	389	1007	1618	635	927	1986	618	3070	472	840	859	164	490	605	1129	0	234	1669	751	3690
G21	1122	433	857	1173	171	725	1536	803	1179	1900	820	3167	533	497	674	221	563	777	1065	234	0	1645	985	3787
G22	948	1208	1774	924	1565	1342	557	1252	1896	809	1756	1952	2066	1509	1087	1803	2095	1218	580	1669	1645	0	1922	2572
G23	1098	1031	186	1236	1139	1600	2020	746	508	2450	173	3593	959	1540	1345	925	921	709	1492	751	985	1922	0	4213
G24	3162	3258	3989	3153	3707	3403	2529	3507	4131	1792	4008	620	4102	3488	3165	3812	4125	3470	2640	3690	3787	2572	4213	0

Table 3
Sugar cane capacity, ton/year.

Province	Capacity
Tucumán	12,220,000
Jujuy	4,324,000
Salta	2,068,000
Santa Fe	125,960
Misiones	62,040

Table 4
Minimum and maximum production capacities of each technology (ton 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 5
Parameters used to evaluate the capital cost for different production technologies.

	α^{PL}_{pgt}, $	β^{PL}_{pgt}, $ year/ton
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 6
Parameters used to evaluate the capital cost for different storage technologies.

	α^{S}_{sgt}, $	β^{S}_{sgt}, $ year/ton
S1	1,220,000	122
S2	18,940,000	1894

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 it is stated in Eq. (20):

$$NE_t = (1-\varphi)(Rev_t - FOC_t - TOC_t) + \varphi DEP_t \quad \forall t \tag{20}$$

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

Table 7
Prices of final products.

	Price, $/ton
White sugar [a]	734
Raw sugar [b]	615
Ethanol [c]	598

[a] No. 407 LIFFE white sugar futures contract
[b] No. 11 ICE raw sugar futures contract
[c] QE NYMEX ethanol futures contract

Table 8
Parameters used to calculate the capital and operating cost for different transportation modes.

	Heavy truck	Lorry	Tanker truck
Average speed (km/h)	55	60	60
Capacity (ton/trip)	30	25	20
Availability of transportation mode (h/day)	18	18	18
Cost of establishing transportation mode ($)	90,000	65,000	100,000
Driver wage ($/h)	10	10	10
Fuel economy (km/L)	5	5	5
Fuel price ($/L)	0.85	0.85	0.85
General expenses ($/day)	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

(PR_{igt}):

$$Rev_t = \sum_{i \in SEP} \sum_{g} DTS_{igt} PR_{igt} \quad \forall t \tag{21}$$

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

$$FOC_t = \sum_{i} \sum_{g} \sum_{i \in IM(p)} UPC_{ipgt} PE_{ipgt} + \sum_{i} \sum_{g} \sum_{i \in IS(s)} USC_{isgt} AIL_{igt} + DC_t \quad \forall t \tag{22}$$

Table 9
Comparison of "full space" method and "rolling horizon" approach.

Case	"Full space" solution	CPU [a]	"Rolling horizon" approach								
			0% [b]	CPU	Error	0.5% [c]	CPU	Error	1% [d]	CPU	Error
2	364,855,004	249	355,681,928	165	2.514%	355,681,928	159	2.514%	355,681,928	133	2.514%
3	748,077,521	190	737,299,005	137	1.441%	747,059,134	110	0.136%	747,059,134	71	0.136%
4	1,103,078,130	387	1,102,408,378	420	0.061%	1,100,709,014	254	0.215%	1,072,612,733	122	2.762%
5	1,488,103,667	975	1,481,385,696	428	0.451%	1,473,161,834	285	1.004%	1,481,093,288	56	0.471%
6	1,800,100,718	4,915	1,793,499,301	880	0.367%	1,794,272,262	378	0.324%	1,792,417,632	110	0.427%
7	2,073,908,387	14,468	2,065,178,757	1996	0.421%	2,066,786,891	687	0.343%	2,071,299,494	128	0.126%
8	2,382,730,430	27,608	2,372,869,869	2548	0.414%	2,373,873,363	702	0.372%	2,370,793,357	345	0.501%
9	2,599,013,033 [e]	43,200	2,591,023,707	7,140	0.487%	2,574,336,476	1,928	1.128%	2,592,387,982	455	0.435%
10	2,790,699,079 [e]	43,200	2,791,675,712	3,637	0.356%	2,785,727,849	2,415	0.569%	2,756,152,808	308	1.624%

[a] CPU time in seconds.
[b] Solution calculated by the "rolling-horizon" method solving the sub-problems with 0% of optimality gap.
[c] Solution calculated by the "rolling-horizon" method solving the sub-problems with 0.5% of optimality gap.
[d] Solution calculated by the "rolling-horizon" method solving the sub-problems with 1% of optimality gap.
[e] Best integer solution after 12 h.

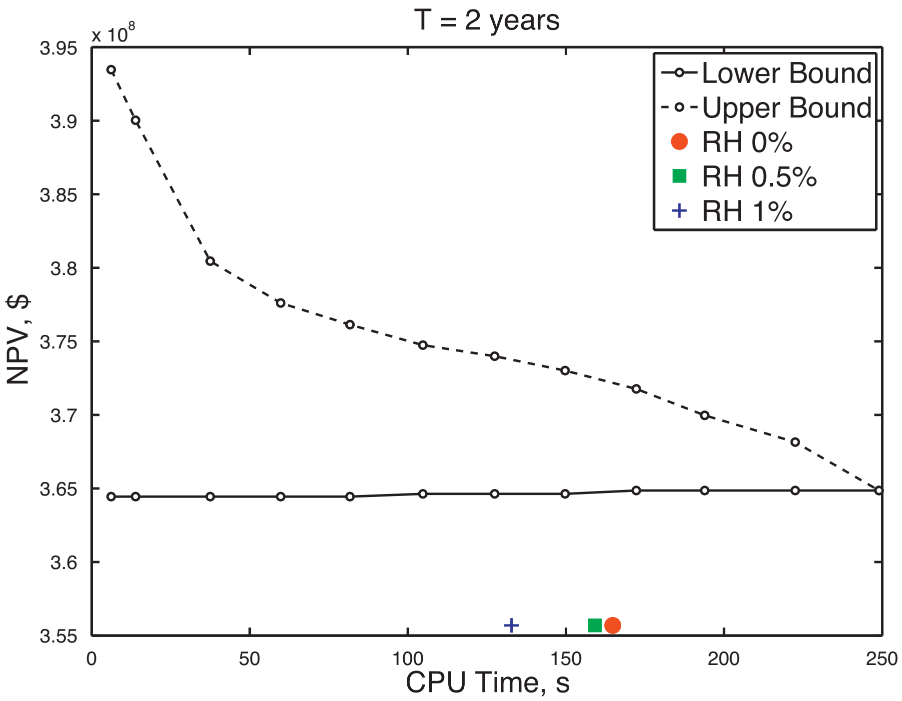

Fig. 4. Comparison of "full space" method vs. "rolling horizon" algorithm (for different optimality gaps imposed on the sub-problems) applied to a two-time-period problem.

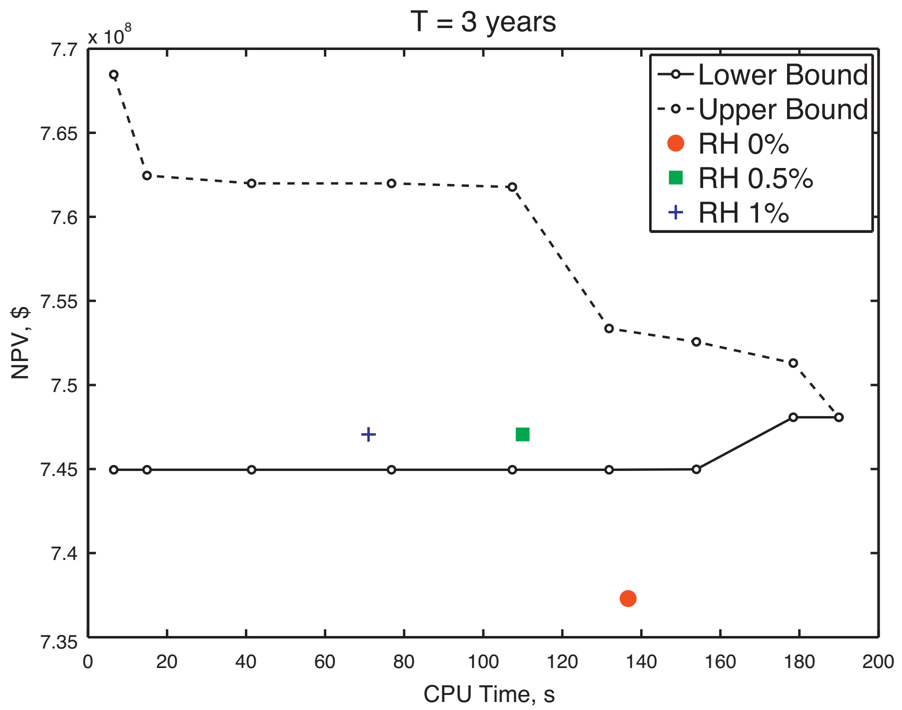

Fig. 5. Comparison of "full space" method vs. "rolling horizon" algorithm (for different optimality gaps imposed on the sub-problems) applied to a three-time-period problem.

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

$$DC_t = \sum_i \sum_g W_{igt} LT_{ig} \quad \forall t \tag{23}$$

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

$$TOC_t = FC_t + LC_t + MC_t + GC_t \quad \forall t \tag{24}$$

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

$$FC_t = \sum_g \sum_{g' \neq g} \sum_l \sum_{i \in IL(l)} \left[\frac{2EL_{gg'} Q_{ilgg't}}{FE_l TCap_l} \right] FP_{lt} \quad \forall t \tag{25}$$

In Eq. (25), the fractional term represents the fuel usage, and 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 ($Q_{ilgg't}/TCap_l$). Note that this equation

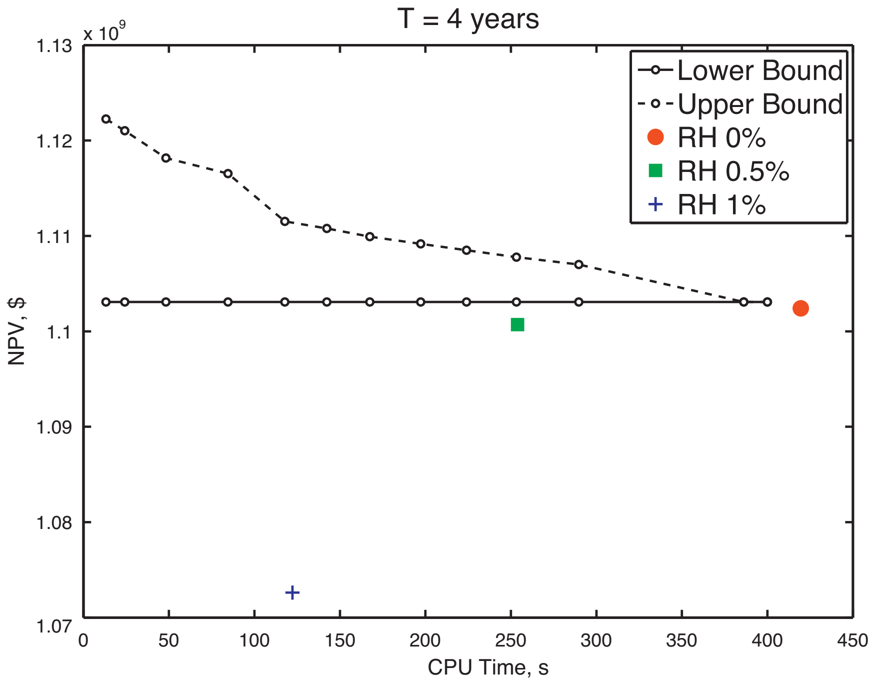

Fig. 6. Comparison of "full space" method vs. "rolling horizon" algorithm (for different optimality gaps imposed on the sub-problems) applied to a four-time-period problem.

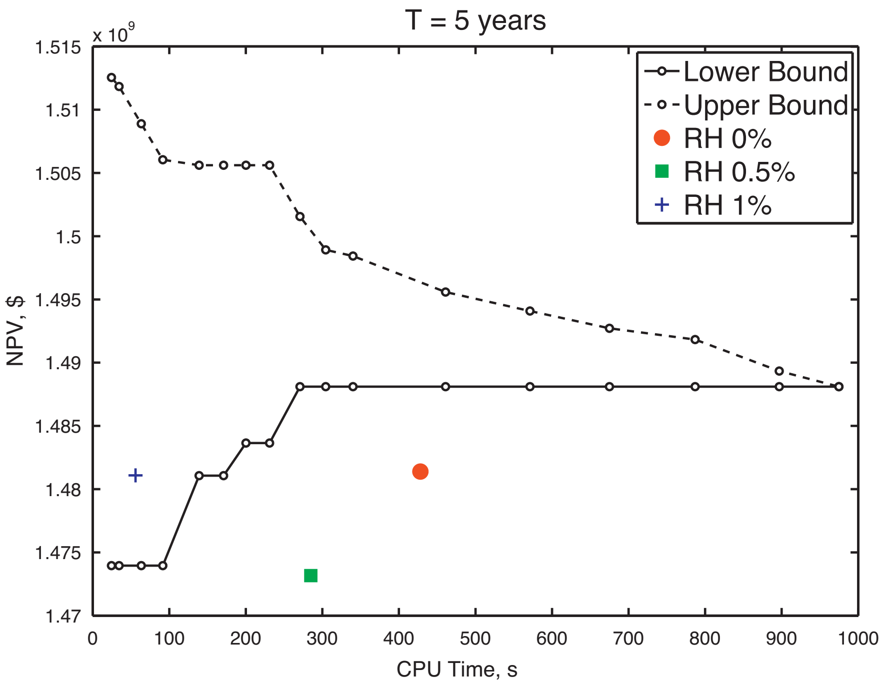

Fig. 7. Comparison of "full space" method vs. "rolling horizon" algorithm (for different optimality gaps imposed on the sub-problems) applied to a five-time-period problem.

assumes that the transportation units operate only between two predefined sub-regions. Furthermore, as shown in Eq. (26), the labor transportation cost is a function of the driver wage (DW_{lt}) and total delivery time (term inside the brackets):

$$LC_t = \sum_g \sum_{g' \neq g} \sum_l DW_{lt} \sum_{i \in IL(l)} \left[\frac{Q_{ilgg't}}{TCap_l} \left(\frac{2EL_{gg'}}{SP_l} + LUT_l \right) \right] \quad \forall t \qquad (26)$$

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

$$MC_t = \sum_g \sum_{g' \neq g} \sum_l \sum_{i \in IL(l)} ME_l \frac{2EL_{gg'} Q_{ilgg't}}{TCap_l} \quad \forall t \qquad (27)$$

Finally, the general cost includes the transportation insurance, license and registration, and outstanding finances. It can be deter-

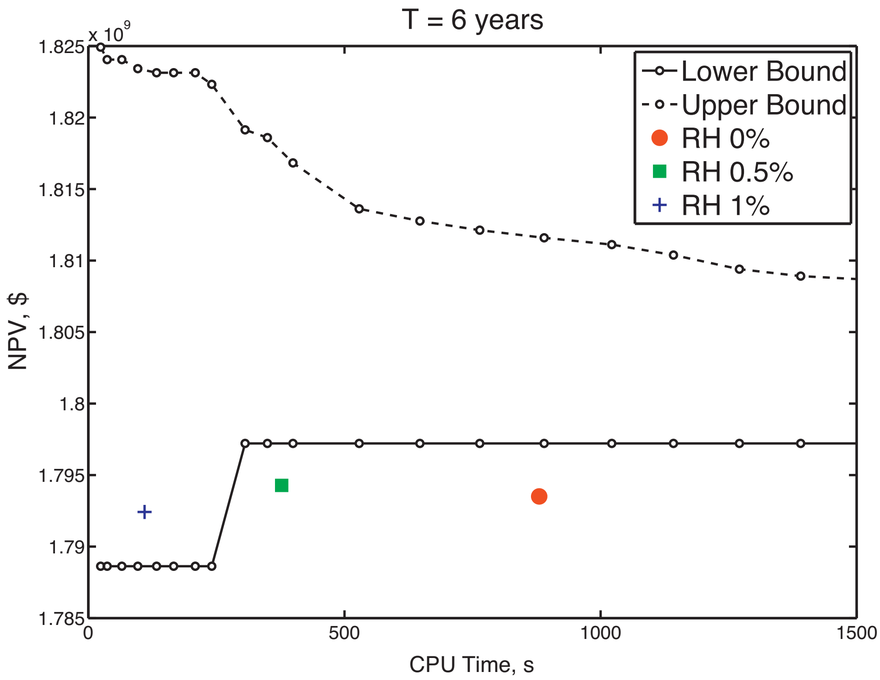

Fig. 8. Comparison of "full space" method vs. "rolling horizon" algorithm (for different optimality gaps imposed on the sub-problems) applied to a six-time-period problem.

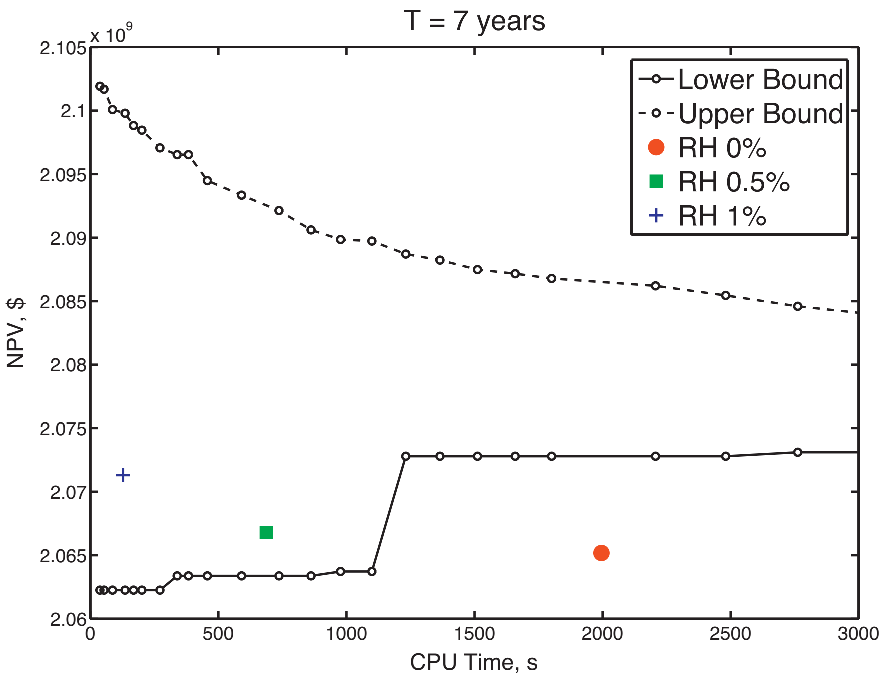

Fig. 9. Comparison of "full space" method vs. "rolling horizon" algorithm (for different optimality gaps imposed on the sub-problems) applied to a seven-time-period problem.

mined from the unit general expenses (GE_{lt}) and number of transportation units (NT_{lt}), as follows:

$$GC_t = \sum_{l} \sum_{t' \le t} GE_{lt} NT_{lt'} \quad \forall t \tag{28}$$

The depreciation term is calculated with the straight-line method:

$$DEP_t = \frac{(1 - sv)FCI}{T} \quad \forall t \tag{29}$$

where FCI denotes the total fixed cost investment, which is determined from the capacity expansions made in plants and warehouses as well as the purchases of transportation units during the

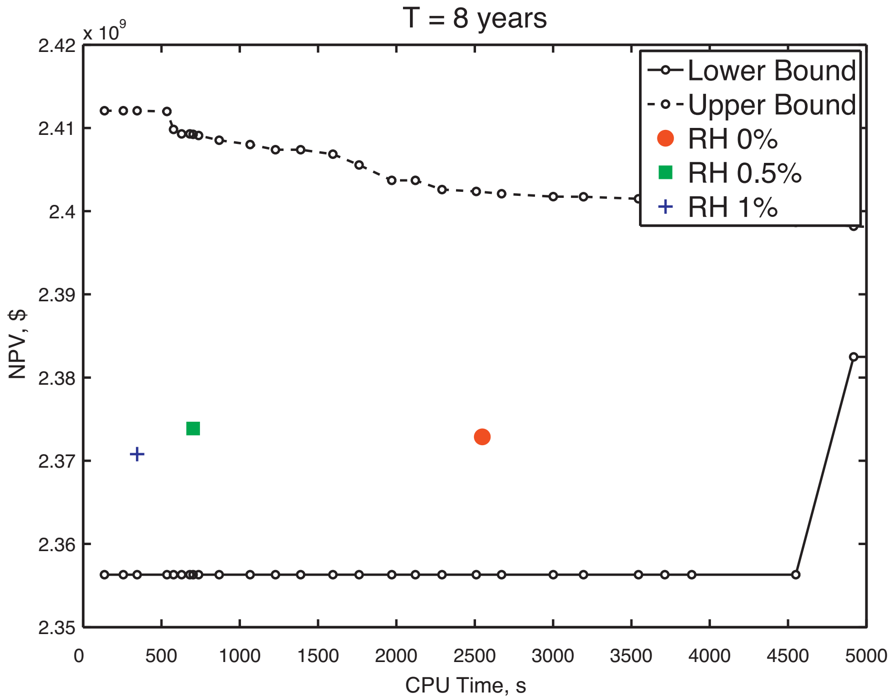

Fig. 10. Comparison of "full space" method vs. "rolling horizon" algorithm (for different optimality gaps imposed on the sub-problems) applied to an eight-time-period problem.

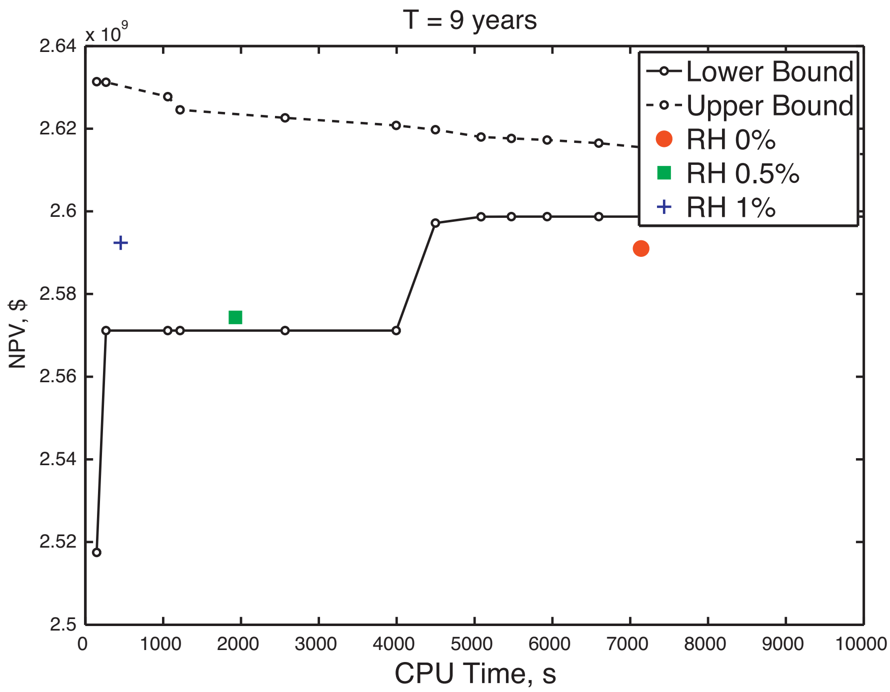

Fig. 11. Comparison of "full space" method vs. "rolling horizon" algorithm (for different optimality gaps imposed on the sub-problems) applied to a nine-time-period problem.

entire time horizon as follows:

$$FCI = \sum_p \sum_g \sum_t (\alpha^{PL}_{pgt} NP_{pgt} + \beta^{PL}_{pgt} PCapE_{pgt}) + \sum_s \sum_g \sum_t (\alpha^{S}_{sgt} NS_{sgt} + \beta^{S}_{sgt} SCapE_{sgt}) + \sum_l \sum_t (NT_{lt} TMC_{lt}) \quad (30)$$

Here, the parameters α^{PL}_{pgt}, β^{PL}_{pgt} and α^{S}_{sgt}, β^{S}_{sgt} 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 to satisfy a certain flow between different sub-regions is computed from the flow rate of products between the sub-regions, the transportation mode availability (avl_l), the capacity of a transport container, the average distance traveled between the sub-regions, the average speed, and the loading/unloading time, as

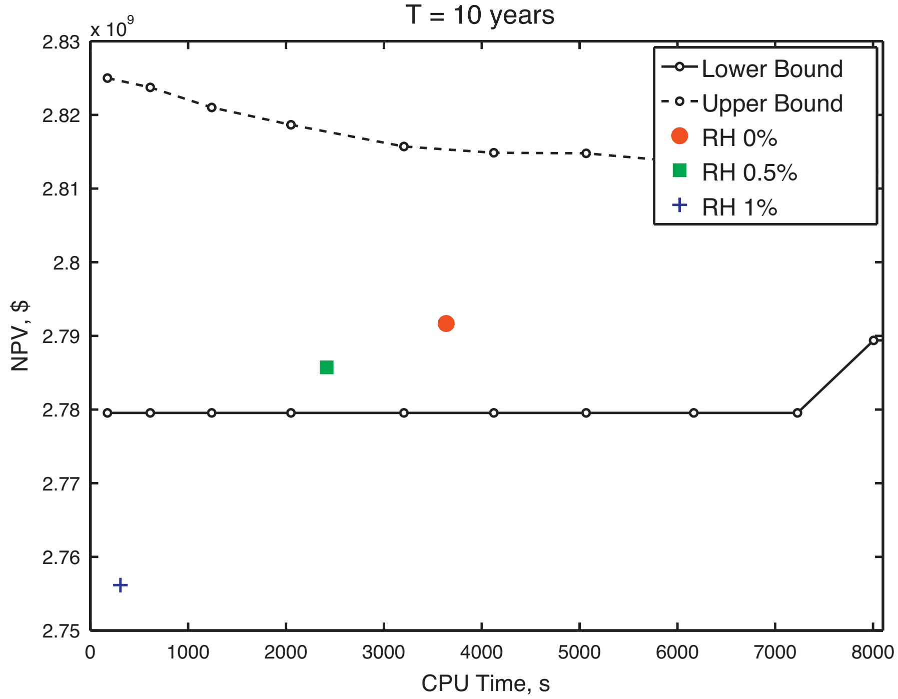

Fig. 12. Comparison of "full space" method vs. "rolling horizon" algorithm (for different optimality gaps imposed on the sub-problems) applied to a ten-time-period problem.

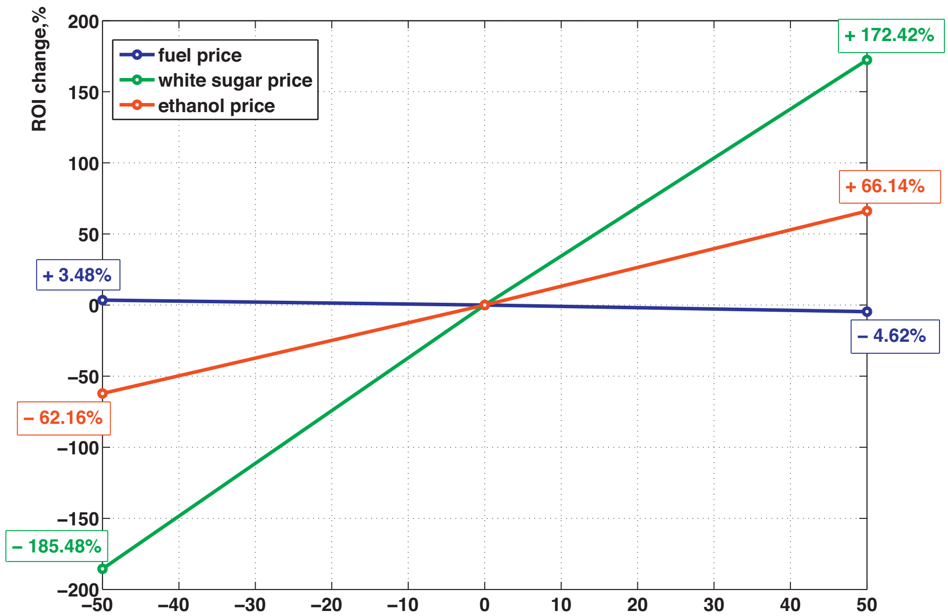

Fig. 13. Influence of fuel, sugar and ethanol prices on ROI.

stated in Eq. (31):

$$\sum_{t \le T} NT_{lt} \ge \sum_{i \in IL(l)} \sum_{g} \sum_{g' \ne g} \sum_{t} \frac{Q_{ilgg't}}{avl_l TCap_l} \left(\frac{2EL_{gg'}}{SP_l} + LUT_l \right) \quad \forall l \tag{31}$$

The total amount of capital investment can be constrained to be lower than an upper limit, as stated in Eq. (32):

$$FCI \le \overline{FCI} \tag{32}$$

Finally, the model assumes that the depreciation is linear over the time horizon. Thus, the depreciation term ($FTDC_t$) is calculated as follows:

$$FTDC_t = \frac{FCI}{T} \quad \forall t \tag{33}$$

Finally, the overall MILP formulation is stated in compact form as follows:

$$\max_{x,X,N} NPV(x, X, N) \qquad \text{(P)}$$

$$\text{s.t. constraints } 1\text{–}33$$

$$x \subset \mathbb{R}, \quad X \subset \{0, 1\}, \quad N \subset \mathbb{Z}^{+}$$

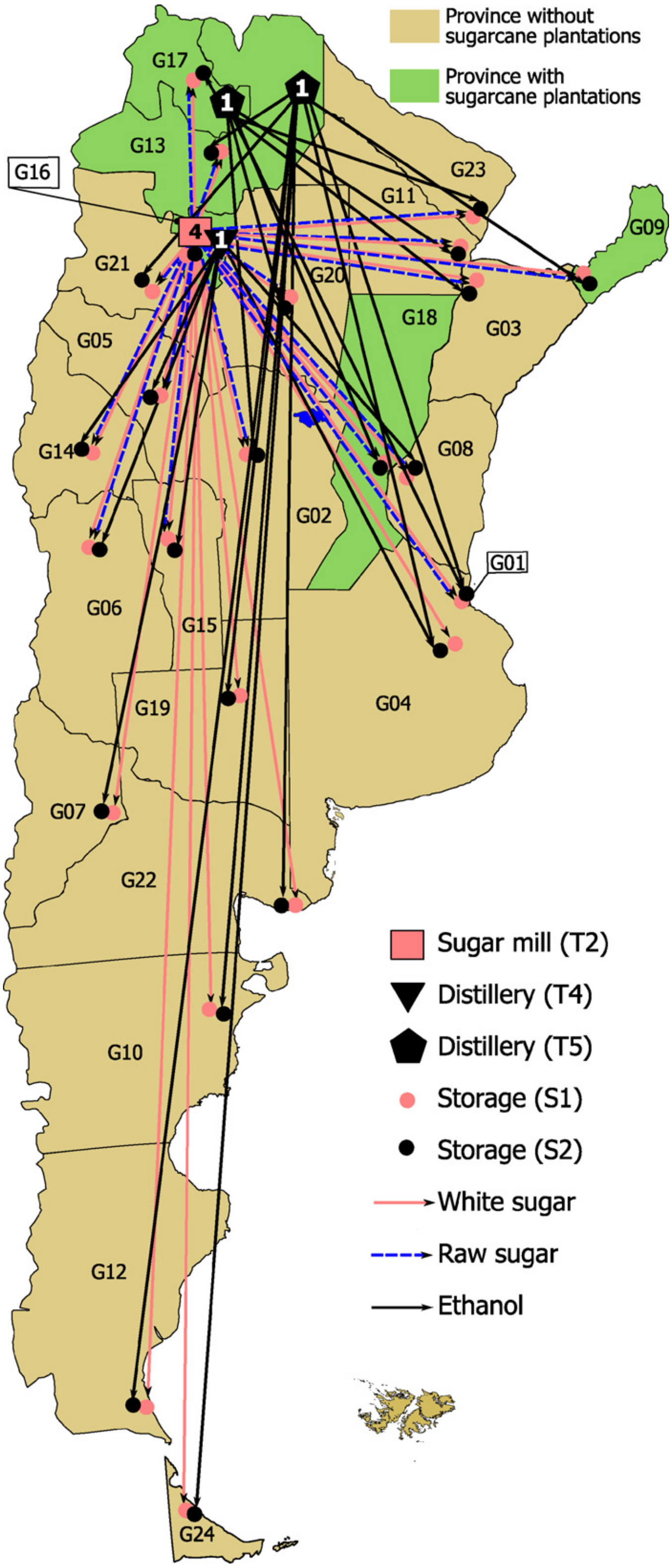

Fig. 14. Configuration of SC under base level of prices, high level of sugar price, low level of ethanol price, and all levels of fuel price.

Here, *x* 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* is the set of integer variables denoting the number of plants, storage facilities and transportation units of each type selected.

The section that follows describes how the MILP problem described above can be efficiently solved via a customized rolling horizon algorithm, thus expediting the overall search for SC configurations that yield large *ROI* values.

4. Solution approach

As shown in the previous section, the MILP model includes decision variables of different nature. The variables which represent the number of production and storage facilities to be installed (NP_{gpt} and NS_{sgt}, respectively) and number of transport modes purchased (NT_{lt}) are integer. Variables $X_{lgg't}$ denoting the existence of transportation links between sub-regions are binary, whereas the remaining variables are continuous. The overall MILP formulation can be solved via branch-and-bound techniques. The complexity of this MILP is mainly given by the number of integer and binary variables, which in our case increases with the number of time periods and sub-regions. Large-scale problems can therefore lead to branch-and-bound trees with a prohibitive number of nodes thus making the MILP computationally intractable. A decomposition method is presented next to reduce the computation burden of the model and facilitate the solution of problems of large size that might be found in practice.

The approach presented is based on a "rolling horizon" scheme (Balasubramanian & Grossmann, 2004; Dimitriadis et al., 1997; Elkamel & Mohindra, 1999), and consists of decomposing the original problem (P) into a number of smaller sub-problems that are solved in a sequential way. A typical "rolling horizon" algorithm relies on an approximate model (i.e., simplification of the original problem) that is formulated for the entire horizon of *T* time periods. In the first iteration, this model is solved providing decisions for the entire horizon, but only those belonging to the first time period are implemented. In the next iteration, the state of the system is updated, and another approximate model is solved for the remaining $T-1$ time periods, freezing the decisions of the first time period already solved. The algorithm proceeds in this manner until all the decisions of the entire time horizon are calculated.

The traditional "rolling horizon" approach relies on solving a sequence of sub-problems of fixed length. This method is not directly applicable to our problem, mainly because there are constraints in our model that impose conditions that must be satisfied over the entire time horizon. Furthermore, the *NPV* calculation requires information from different time periods, which makes it difficult to implement the traditional "rolling horizon approach.

Particularly, to derive the approximate models used by our "rolling horizon" strategy, we exploit the fact that the relaxation of the integer variables of the full space formulation (P) is very tight. In other words, the solution that is obtained when (P) is solved defining *NP*, *NS*, and *NT* as continuous variables rather than as integers, is very close to the optimal solution of the original problem. The reason for this is that in practice these integer variables take large values, since they represent the number of facilities to be established in big regions that cover high demands.

Hence, the approximate models of our algorithm are constructed by relaxing the integer variables denoting the number of transportation units and production and storage facilities established in periods beyond the first one. The motivation behind this

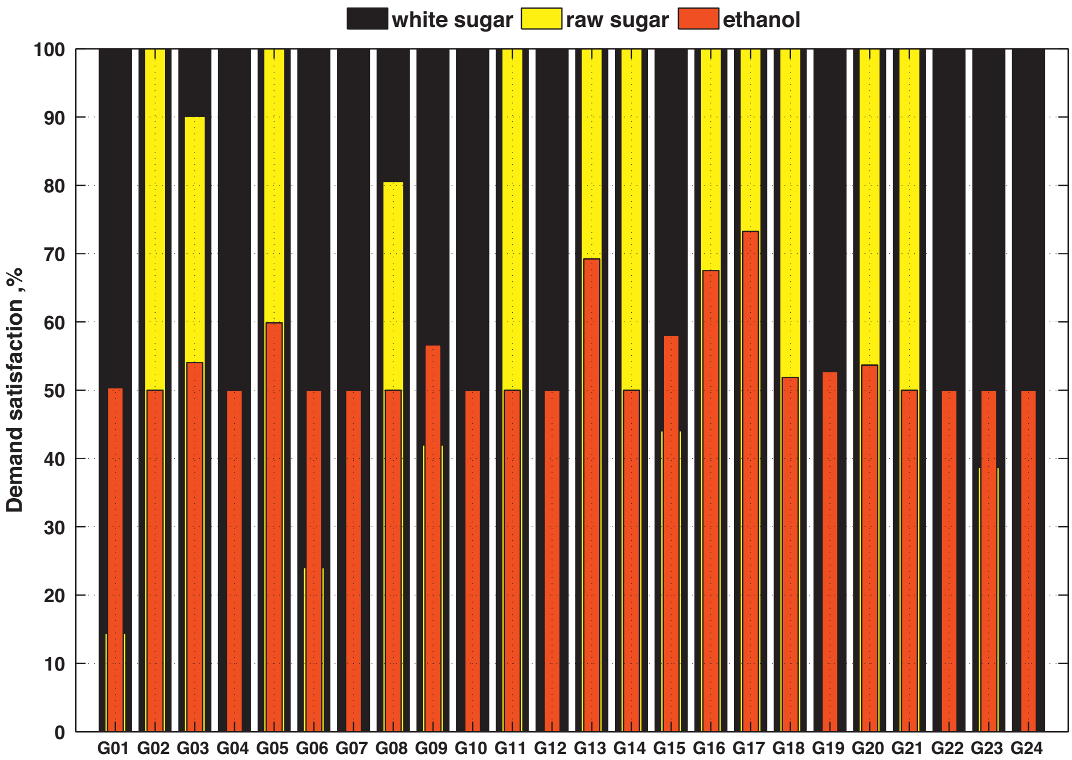

Fig. 15. Demand satisfaction level under base level of prices and high level of sugar prices.

procedure is that the computational complexity is greatly reduced by dropping the integrality requirement on these variables without sacrificing too much the quality of the solution. Therefore, in each iteration the method concentrates on determining the values of the integer variables of one single period, whereas the relaxed part of the problem allows to assess in an approximate manner the effect that these decisions have on later periods. The solutions of these sub-problems, all of which are relaxations of the original full space model (P), are then used to approximate the optimal solution of (P). Each sub-problem (AP) can therefore be expressed as follows:

$$\max_{x,X,N} NPV(x, X, N) \qquad \text{(AP)}$$
$$\text{s.t. constraints } 1\text{–}33$$
$$N = (N' \cup RN)$$
$$x \subset \mathbb{R}, \quad RN \subset \mathbb{R}, \quad X \subset \{0, 1\}, \quad N' \subset \mathbb{Z}^+$$

where $N' = (NP_{pgt'}, NS_{sgt'}, NT_{lt'})$ denotes the vector of integer variables corresponding to time period t' and $RN = (RNP_{pgt}, RNS_{sgt}, RNT_{lt})$ is the vector of continuous variables representing the strategic decisions associated with those time intervals beyond t' (i.e. $t > t'$). The "rolling horizon" algorithm proposed in this work is as follows:

1. **Initialization**.
   Set iteration counter (*ctr*) equal to 1.
   Go to step 2.
2. **Solution**.
   Solve the subproblem (AP) with the branch-and-bound method relaxing the variables corresponding to those periods beyond *ctr*.
   Fix the variables for time interval $t = ctr$.
3. **Termination check**.
   If $ctr < T$, then set $ctr = ctr + 1$ and go to step 2.
   Otherwise, there are no more sub-problems to be solved (termination).

Fig. 3 illustrates the way in which the algorithm would proceed for a problem with 4 time periods. Note that the time horizon of each approximate sub-problem is divided into two time blocks:

1. The "integer block", which covers the first period of the sub-problem and in which all the integer decision variables NP_{pgt}, NS_{sgt} and NT_{lt} remain unchanged. Note that this first interval moves forward as iterations proceed.
2. The "relaxed block", which comprises all the periods beyond the current one, in which the integer variables denoting the number of production plants, storage facilities and transportation units are relaxed into continuous variables RNP_{pgt}, RNS_{sgt} and RNT_{lt}, respectively.

Remarks

- Before implementing the decomposition strategy, it is convenient to check the tightness of the integer relaxation of the model for small instances of the problem. If the relaxation is not tight enough, the method is not likely to work properly. In this case, alternative methods can be used (see Guillén-Gosálbez et al., 2010).
- The sub-problems can be constructed by relaxing only some of the integer variables instead of all of them. To choose the variables to be relaxed, one can perform a preliminary analysis in order to assess the impact of relaxing the variable on the CPU time and quality of the relaxation.

- The complexity of the model grows with the number of time periods, sub-regions and technologies. By merging neighboring sub-regions with low and high demands one can reduce the overall complexity of the model.
- It is not necessary to solve the sub-problems of the rolling-horizon method to global optimality. In fact, the overall method can be expedited by solving the sub-problems (AP) for low optimality gaps (i.e., less than 5%). This reduction in CPU time might be achieved at the expense of compromising the quality of the final solution.

5. Case study

In order to illustrate the capabilities and advantages of the proposed approach, a case study based on the sugar cane industry of Argentina was solved, comparing the results obtained by the full space branch-and-bound method with those reported by the approximate algorithm.

The problem consists of 24 sub-regions representing original Argentinean provinces with corresponding demand of sugar and ethanol. The sub-regions and demand values corresponding to the first time period are shown in Table 1, whereas the demand for the remaining periods is provided as supplementary material. Distances between sub-regions were determined considering the capitals of the corresponding provinces and the main roads connecting these capitals. These data are listed in Table 2.

We assume that each sub-region has an associated sugar cane capacity. Particularly, sugar cane plantations are situated in five Argentinean provinces, whose production capacities are given in Table 3. The remaining regions have the option of importing sugar cane from these provinces, which may eventually lead to an increase in the transport operating cost. The minimum and maximum production capacities of each technology are listed in Table 4. The minimum and maximum storage capacities for liquid and solid materials are assumed to be 200 and 2 billion tons, respectively. The unit storage cost is assumed to be \$0.365/(ton year) for all types of materials. Fixed and variable investment coefficients for different production and storage modes are listed in Tables 5 and 6, respectively. The prices for final products obtained from actual trading data are presented in Table 7. Unit production cost for sugar and ethanol are equal to \$265/ton and \$317/ton, respectively. The parameters used to calculate the capital and operating cost for different transportation modes can be found in Table 8. The minimum flow rate of each transportation mode is assumed to be equal to the minimum capacity of the corresponding transportation mode, whereas the maximum flow rates for heavy trucks, medium trucks and tanker trucks are 6.25, 6.25 and 6.00 million tons per year, respectively.

5.1. *Computational performance of the "rolling horizon" approach as compared to the NPV-based MILP*

To highlight the computational performance of the proposed "rolling horizon" algorithm as compared to a "full space" branch-and-bound method, nine example problems were solved maximizing *NVP* as single objective. Because the issue is to highlight the computational advantages, there is no need to apply the overall heuristic method to maximize the *ROI*.

The problems to be solved had different levels of complexity based on the length of the time horizon. All the models were written in GAMS (Rosenthal, 2008) and solved with the MILP solver CPLEX 12 on a HP Compaq DC5850 desktop PC with an AMD Phenom 8600B, 2.29 GHz triple-core processor, and 2.75 Gb of RAM.

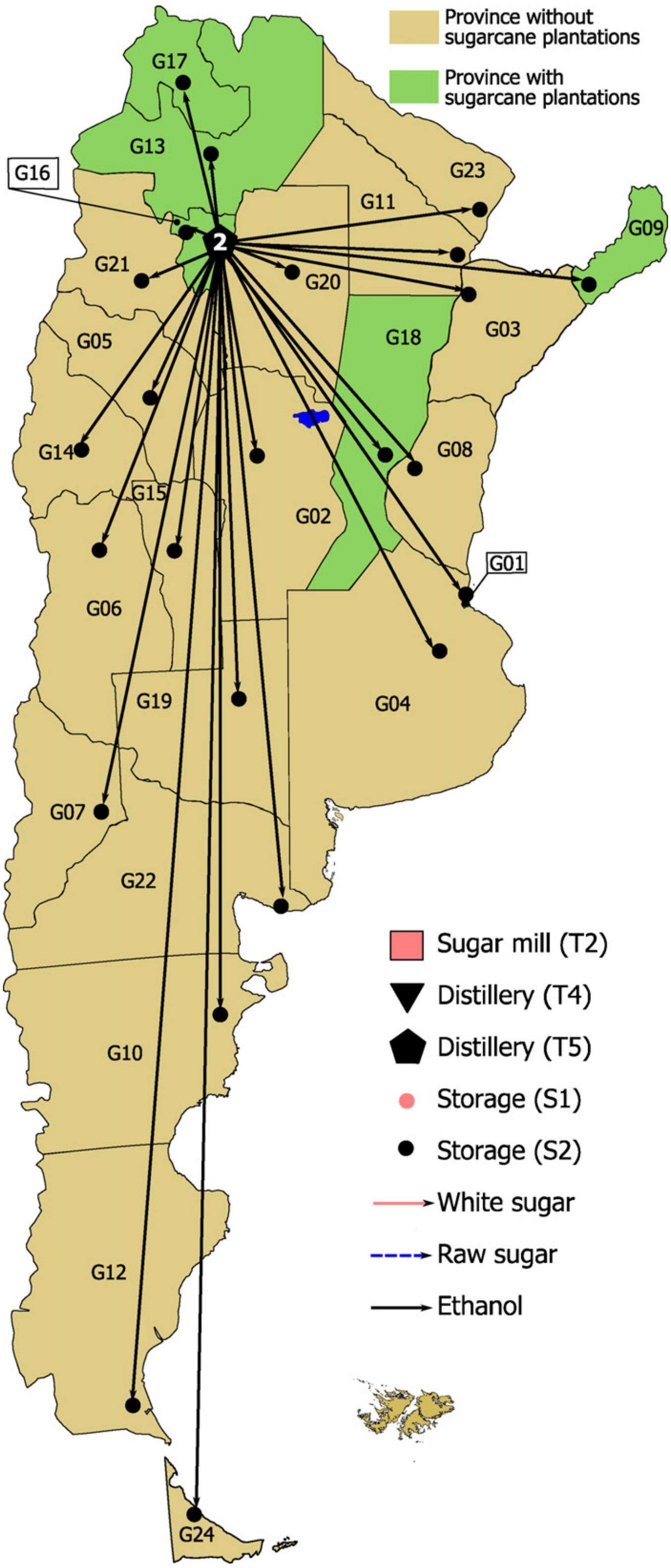

Fig. 16. Configuration of SC under low level of white sugar price.

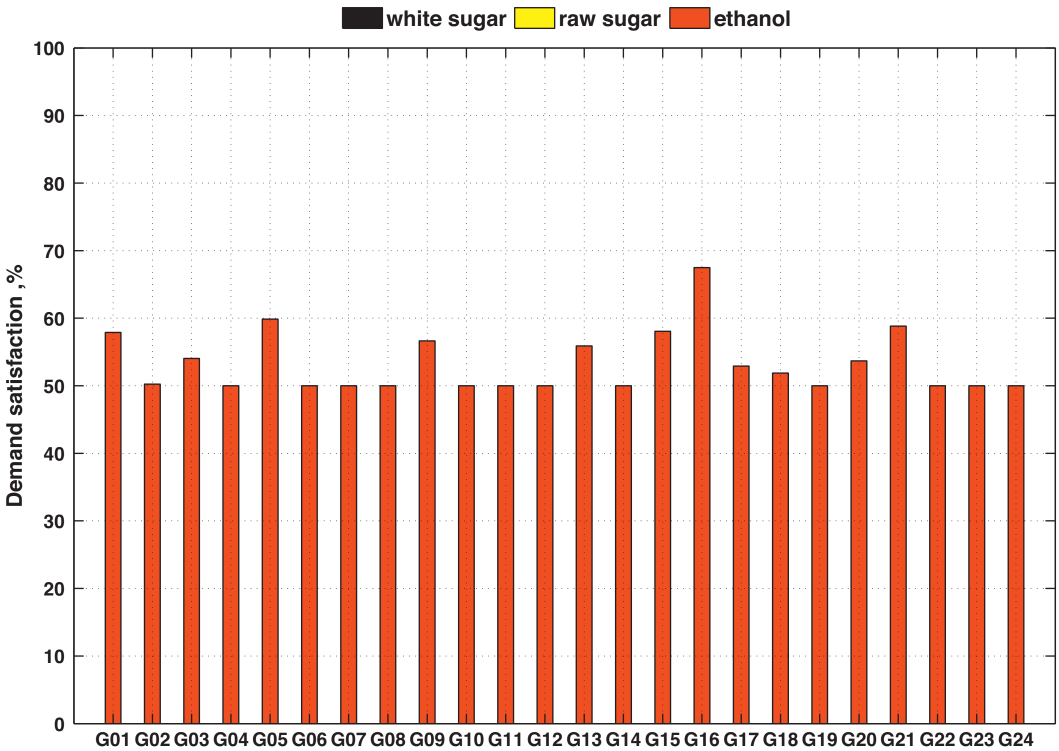

Fig. 17. Demand satisfaction level under low level of sugar price.

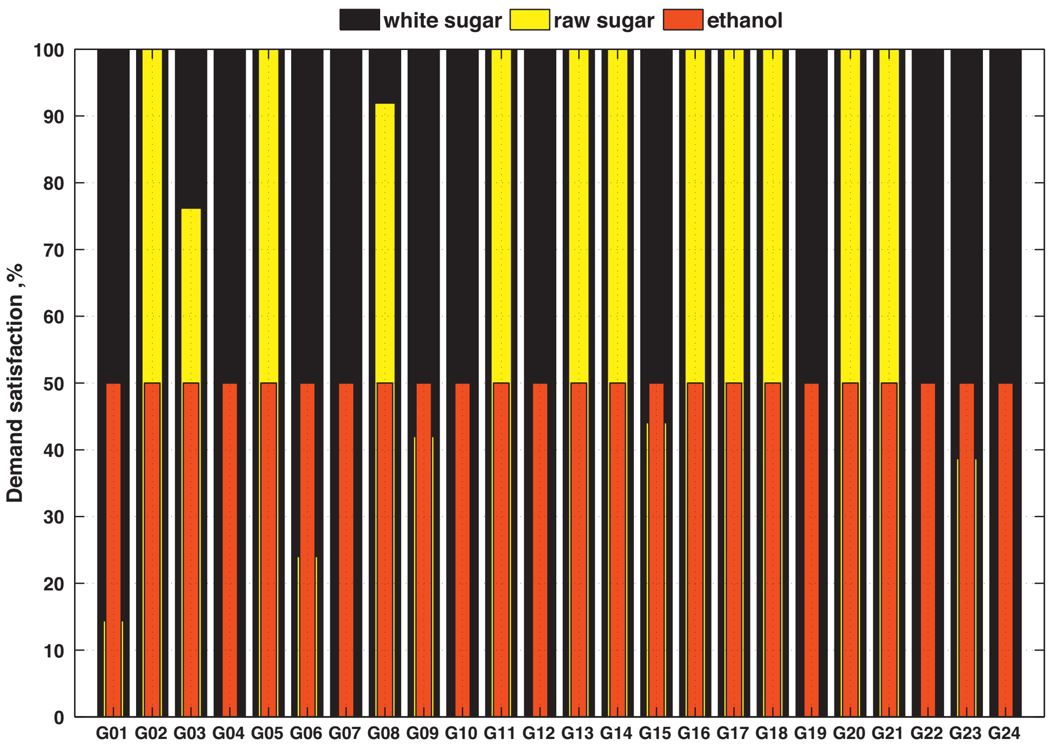

Fig. 18. Demand satisfaction level under low level of ethanol price.

Specifically, the “full space” and “rolling horizon” methods were applied to several problems with time horizons from 2 to 10 years. The upper bound on the capital investment was 1.5 billion $ for all of them.

Figs. 4–12 show the lower and upper bounds provided by the “full space” method as a function of time. In the same figures, we have depicted the solutions calculated by the “rolling-horizon” algorithm using different optimality gaps in the sub-problems. As

Table 10
Capital investments utilized with maximum ROI.

Case	FCI, $	NPV, $	ROI
Base level	1.77×10^9	479,217,967	0.1081
High ethanol price	1.86×10^9	868,467,640	0.1796
Low ethanol price	1.74×10^9	151,473,075	0.0409
High sugar price	1.77×10^9	1,375,331,563	0.2945
Low sugar price	1.10×10^9	−297,129,603	−0.0924
High fuel price	1.77×10^9	455,791,162	0.1031
Low fuel price	1.79×10^9	503,390,346	0.1119

seen, for 2 and 4 time periods, the “full space” method performs better than the rolling horizon, whereas in the remaining cases, there is always at least one tuning of the “rolling-horizon” algorithm that outperforms CPLEX in terms of time (i.e., our algorithm provides solutions with less than 3% of optimality gap in shorter CPU times).

Table 9 provides the optimal solution (i.e., the solution with zero optimality gap) of each instance being solved along with the solutions calculated by the “rolling-horizon” method solving the sub-problems with different optimality gaps. Note that the model can only be solved to global optimality in some cases, whereas in others it is not possible to close the gap to zero after 43,200 of CPU time. Hence, the optimal results refer either to the global optimal solution (in those cases in which such a solution is identified before the time limit is exceeded) or to the solution attained after 43,200 of CPU time. As observed, the “rolling-horizon” algorithm provides in all the cases solutions with low optimality gaps (less than 3%).

5.2. *Results for the case study*

After proving the computational efficiency of the method, we next used the model to obtain valuable insight on the SC design problem for different plausible scenarios that differ in the cost data. We consider a three-year planning horizon assuming the input data given in Tables 7 and 8. A minimum demand satisfaction level constraint that forces the model to fulfill at least 50% of the ethanol demand in each sub-region was also included. Particularly, we solved the problem for the base case and compared the obtained results with the cases of low (50% below the base case level) and high levels (50% above the base case level) of fuel, sugar and ethanol prices.

For generating solutions close to the maximum *ROI* using our heuristic approach, we divided the interval $[0, \overline{FCI}]$ into 20 subintervals and maximized the *NPV* for different upper bounds on the capital investment that corresponded to the limits of these subintervals. From the obtained solutions, we identified the one with the largest *ROI*. The results of this analysis are presented in Table 10. The resulting *ROI* values for different levels of prices are depicted in Fig. 13.

As shown, ethanol and white sugar prices have the greatest impact on the *ROI* whereas the impact of the fuel price is rather low. The *ROI* and *NPV* take negative values in some cases because the model is forced to attain a minimum demand satisfaction level of ethanol of 50%, even if the production of this product is not profitable. This could be an important result for decision makers, calling for some subsidies or tax relief. Table 11 presents capital and operational expenditures as well as revenues for different prices. As observed, plant, storage and transportation capital costs have similar values. This is due to the small amount of production facilities and large number of storages and transportation links that must be established in the whole territory of Argentina to guarantee a minimum demand satisfaction level for ethanol of 50% in each Argentinean province. Regarding operating cost,

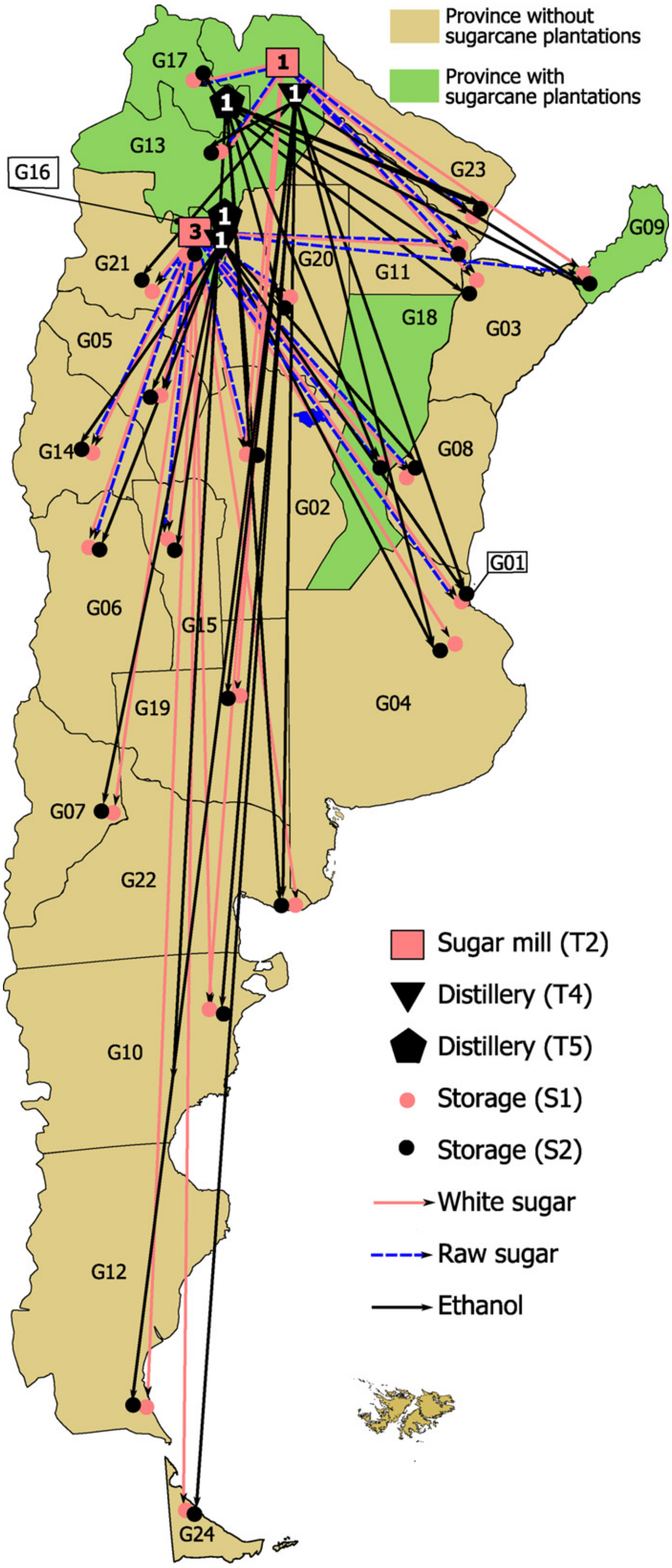

Fig. 19. Configuration of SC under high level of ethanol price.

landfill expenditures have the smallest share in the operating cost for all cases, and facility operating cost is ten times greater than transportation payments. Among the most profitable cases (high level of white sugar and ethanol price and low level of fuel price) the greatest value of revenue occurs with the increased price of white sugar.

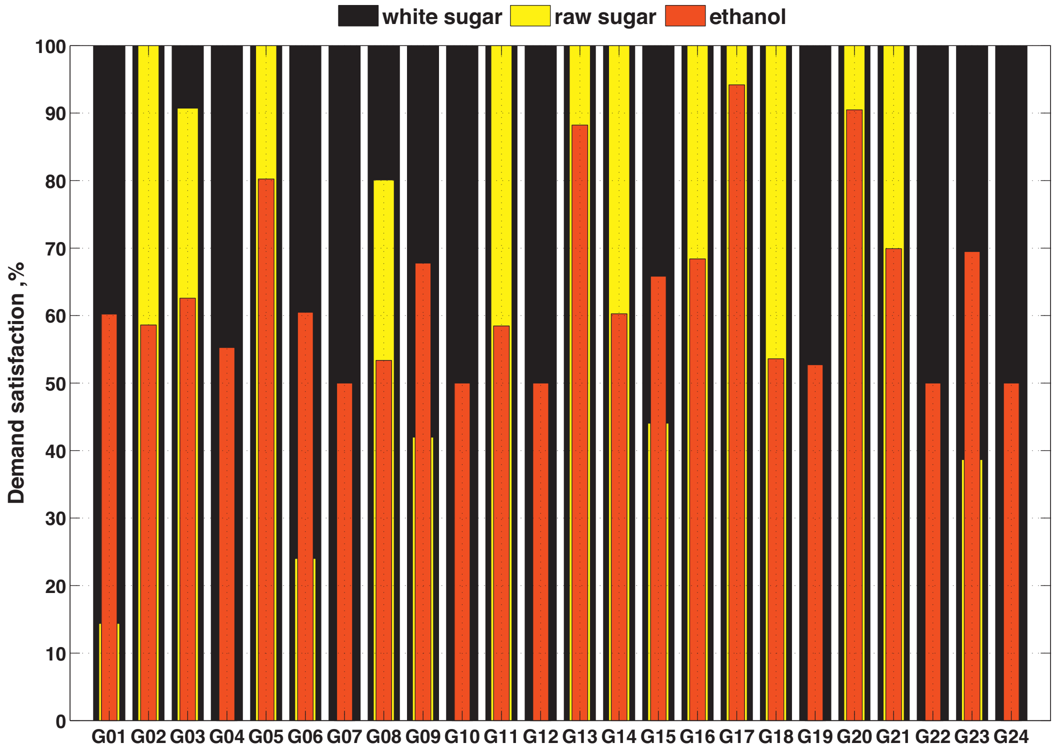

Fig. 20. Demand satisfaction level under high level of ethanol price.

Fig. 14 illustrates the SC configuration for the base case. The absence of sugar cane plantations in most of the Argentinean provinces results in a centralized SC that involves the establishment of production facilities only in Tucumán, Jujuy and Salta, which have inner sources of sugar cane. This configuration is motivated by the large amount of raw materials required for sugar and ethanol production, which would lead to prohibitive transportation cost if the plants were settled far away from the plantations. The resulting demand satisfaction level is shown in Fig. 15. As observed, most of the provinces, except Tucumán and a number of neighboring regions, attain the minimum possible ethanol supply, which indicates the unfavorable situation for ethanol in these regions compared to sugar.

We now show how the model responds to the changes on prices. We illustrate their effect on the optimal SC configuration and the way in which the model can be used to analyze situations that can be encountered in practice. The reduction of sugar price makes the model switch from the combined sugar-ethanol network to an exclusively bioethanol SC with 2 production plants that convert sugar cane directly into ethanol (i.e., distillery T5). The SC configuration for low white sugar price is depicted in Fig. 16. Fig. 17 shows the demand satisfaction level in this case. The need to supply all regions with ethanol and a sugar cane deficit make that ethanol demand is not satisfied completely even in the provinces with their own sugar cane plantations.

The optimal SC configuration for the base level of the product prices remains optimal for the case of the increased sugar price. This happens because the ethanol demand satisfaction constraint results in that sugar cane is converted mainly in ethanol, and sugar factories have not enough amount of raw materials to expand sugar production even under very favorable conditions in the sugar market. Hence, there is no difference in SCs topology and demand satisfaction pattern between the base and high levels of sugar prices.

Fig. 18 depicts the demand satisfaction level under low price of ethanol. It shows that the distilleries produce only the minimum amount of ethanol necessary to attain a 50% of demand satisfaction. For this case the SC configuration is the same as in the base case.

Table 11
Impact of fuel, sugar and ethanol prices on capital and operating costs.

Case	Capital cost, $			Operating cost, $			Revenue,$
	Plants	Storages	Transportation links	Disposal	Facility	Transportation	
Fuel price							
Low level	1,171,823,436	582,485,087	34,160,000	2,482,742	1,478,344,669	173,343,027	3,939,862,440
Base level	1,154,384,264	582,485,087	33,560,000	2,408,644	1,459,984,820	208,941,020	3,905,368,643
High level	1,157,272,391	582,485,087	32,635,000	2,388,156	1,454,908,384	239,818,010	3,895,831,223
Sugar price							
Low level	562,340,000	525,742,524	12,800,000	2,312,061	572,930,061	58,694,929	1,076,400,000
Base level	1,154,384,264	582,485,087	33,560,000	2,408,644	1,459,984,820	208,941,020	3,905,368,643
High level	1,154,384,264	582,485,087	33,560,000	2,408,644	1,459,984,820	208,941,020	5,319,719,295
Ethanol price							
Low level	1,128,335,938	582,210,025	33,560,000	2,297,980	1,432,561,324	207,749,576	3,341,273,840
Base level	1,154,384,264	582,485,087	33,560,000	2,408,644	1,459,984,820	208,941,020	3,905,368,643
High level	1,239,355,122	585,161,472	34,530,000	2,736,842	1,541,324,478	213,160,522	4,672,929,399

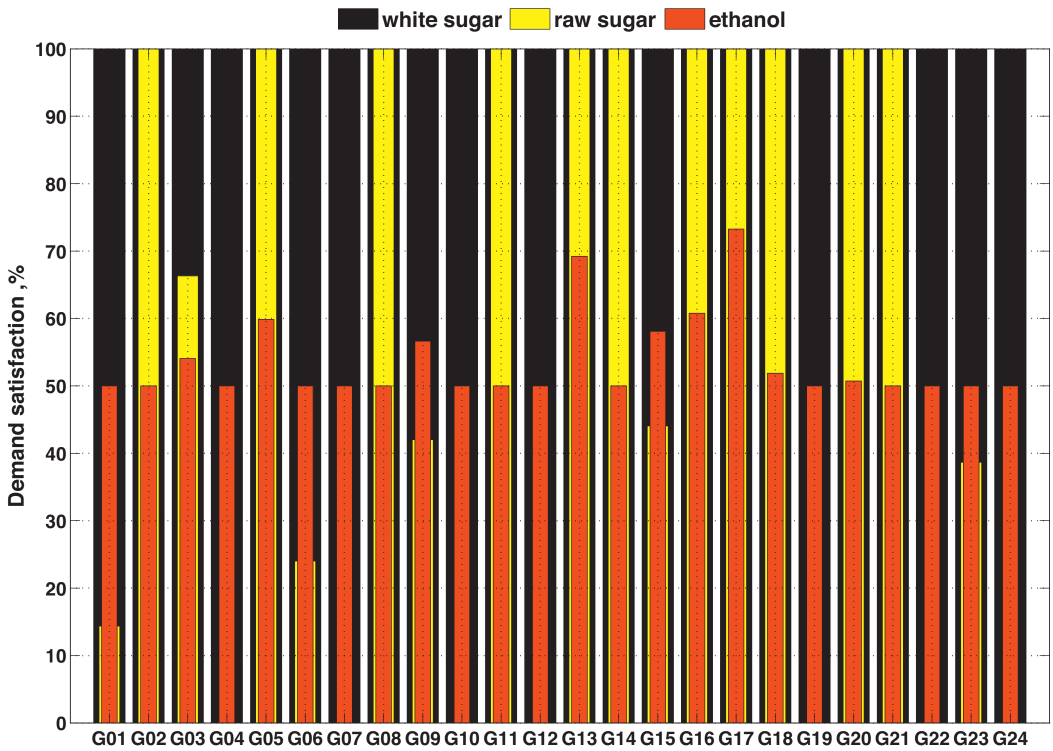

Fig. 21. Demand satisfaction level under high level of fuel price.

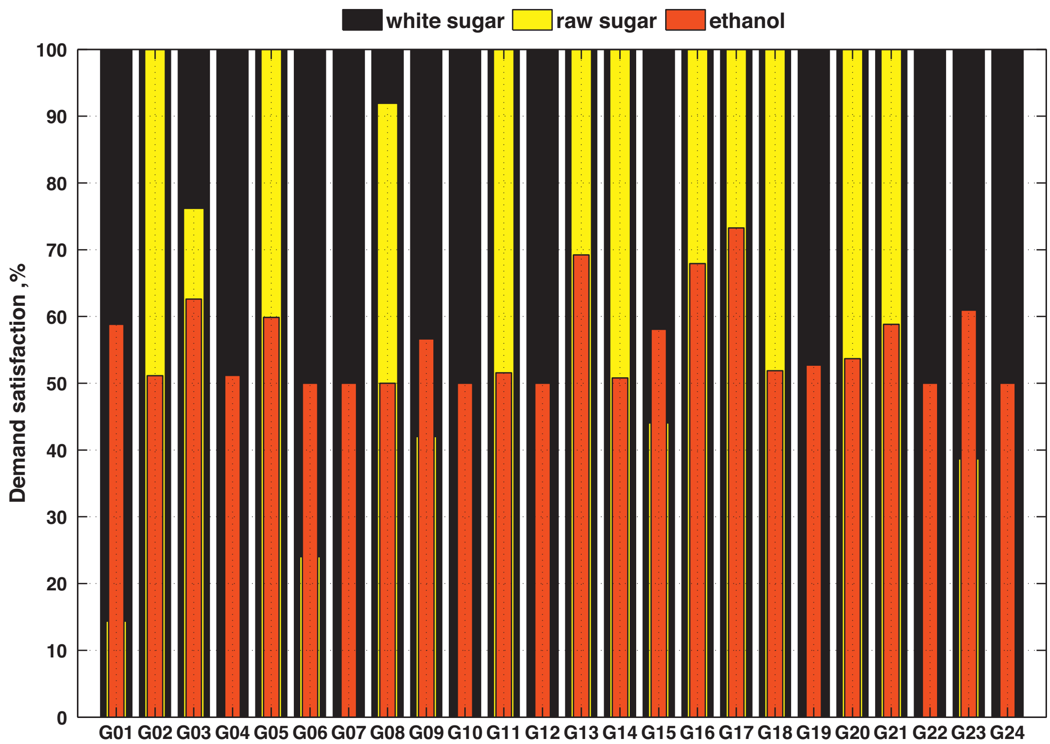

Fig. 22. Demand satisfaction level under low level of fuel price.

On the other hand, a 50% increase in the ethanol price increases the ethanol production and sugar cane consumption and leads to the establishment of a new distillery T5 in Tucumán and a shift from technology T5 to the pair T2–T4 in Salta. The SC configuration under high level of ethanol price is depicted in Fig. 19. Fig. 20 depicts the demand satisfaction level under high level of ethanol price. This plot shows that a 50%-increase of ethanol price results in a significant growth of the demand satisfaction level of ethanol and a shrinkage in sugar production.

With regard to the fuel price, we note that this parameter has the lowest influence on the *NPV*, and its fluctuations mainly result in changes of production capacity but do not affect the supply chain configuration that remains the same as under the base level of prices. Figs. 21 and 22 show the demand satisfaction level under high and low level of fuel price, respectively. As shown, a 50%-decrease of fuel price favors the ethanol production leading to higher ethanol demand satisfaction levels in the distant Argentinean provinces

6. Conclusions

In this work we have addressed the optimal design and planning of integrated sugar/ethanol SCs. The design task was formulated as a mixed-integer programming problem that seeks to maximize the *ROI* and that is approximated by solving a series of MILPs that maximize the *NPV* for different fixed capital investment values. To overcome the large computational burden of solving these MILPs, we proposed an approximation algorithm based on a "rolling horizon" strategy. The capabilities of the proposed mathematical model and solution strategy were shown through a case study based on the Argentinean sugar cane industry.

On the computational side, the "rolling horizon" algorithm provided near optimal solutions (i.e., with less than 3% of optimality gap) in a fraction of the time spent by CPLEX. A sensitivity analysis was also conducted to study the impact that the prices of fuel, ethanol and sugar have on the economic performance and structural configuration of the SC. It was shown that sugar price has the greatest influence on the structure and performance of the integrated ethanol/sugar supply chain. The SC configurations obtained in all the cases are rather centralized, involving the establishment of few production facilities close to the sugar cane plantations. The systematic tool presented in this article aims to facilitate the task of decision makers from the viewpoints of analysis, improvement and optimization of distributed facilities.

Acknowledgments

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Appendix A. Demand data

Sub-region	White sugar	Raw sugar	Ethanol
1st year			
G01	53,644	40,249	60,394
G02	84,280	62,874	108,680
G03	17,848	17,556	31,812
G04	276,077	292,334	342,248
G05	11,647	3038	7860
G06	64,097	11,366	70,309
G07	22,832	5188	19,950
G08	25,634	11,980	38,342
G09	25,365	11,358	30,888
G10	8193	7975	8622
G11	25,587	11,709	31,952
G12	5259	2243	5255
G13	25,889	15,700	33,242
G14	12,074	8440	27,652
G15	17,568	2599	9377
G16	46,365	18,572	79,890
G17	22,286	7753	17,350
G18	62,814	36,975	89,866
G19	10,321	2777	9133
G20	29,559	6875	26,944
G21	10,793	4233	8375
G22	8576	7842	14,485
G23	22,035	5533	19,958
G24	3852	2224	3890
2nd year			
G01	55,458	23,072	107,728
G02	96,928	15,136	66,945
G03	26,914	6959	39,482
G04	690,366	202,816	495,091
G05	13,053	6469	7866
G06	56,074	12,265	62,488
G07	15,706	6748	13,828
G08	24,062	15,149	34,272
G09	36,053	16,195	21,359
G10	17,035	4826	17,895
G11	17,264	10,214	9900
G12	4824	1430	8731
G13	37,737	13,325	23,540
G14	24,968	13,342	26,827
G15	10,067	5931	14,834
G16	24,406	12,927	40,222
G17	18,261	6264	10,412
G18	49,098	34,633	90,737
G19	7760	4845	8755
G20	18,144	5567	28,084
G21	6333	4245	7301
G22	6422	7554	16,559
G23	9620	9249	12,789

Sub-region	White sugar	Raw sugar	Ethanol
G24	3413	1035	2170
3rd year			
G01	59,180	34,173	100,186
G02	88,651	52,658	102,458
G03	32,935	14,046	23,319
G04	618,341	208,166	435,812
G05	10,195	4798	13,662
G06	41,832	27,447	39,005
G07	12,648	6073	15,545
G08	20,107	20,137	35,143
G09	33,125	11,004	43,606
G10	12,678	3800	17,819
G11	19,143	15,705	29,725
G12	4797	2679	4121
G13	32,798	13,881	45,252
G14	15,404	4286	13,037
G15	8660	4931	9591
G16	58,951	14,898	56,302
G17	16,247	8069	14,875
G18	32,433	50,177	100,418
G19	11,106	3864	10,686
G20	20,912	9453	23,443
G21	8316	2965	4763
G22	10,287	6759	14,577
G23	12,048	9136	9165
G24	2971	1430	1782
4th year			
G01	81,041	37,553	106,659
G02	82,537	49,586	142,621
G03	24,431	9003	21,211
G04	452,336	175,920	433,350
G05	10,352	5807	8657
G06	54,661	24,024	20,394
G07	10,726	9004	13,475
G08	22,663	16,499	26,419
G09	49,358	10,011	50,260
G10	12,714	4271	15,163
G11	32,203	11,762	19,996
G12	2335	2065	5685
G13	26,105	20,109	27,515
G14	24,708	7233	23,561
G15	10,183	5466	14,293
G16	36,335	17,611	63,779
G17	25,468	5588	24,870
G18	77,247	48,772	96,126
G19	6889	3701	9886
G20	14,814	8601	13,183
G21	6363	3899	12,756
G22	14,532	4925	20,775

Sub-region	White sugar	Raw sugar	Ethanol
G23	12,865	8755	15,089
G24	4507	1442	548
5th year			
G01	90,436	57,265	45,973
G02	116,148	43,967	75,119
G03	22,863	7206	35,502
G04	527,709	234,621	402,829
G05	12,864	5562	3681
G06	65,022	22,279	49,087
G07	18,420	3426	14,455
G08	36,948	10,959	28,498
G09	23,199	14,015	34,941
G10	12,668	3150	9478
G11	29,923	18,584	43,724
G12	7568	2013	3750
G13	26,388	14,973	27,764
G14	19,210	9292	21,302
G15	10,354	5268	12,824
G16	40,946	26,396	36,171
G17	11,299	7951	12,616
G18	105,312	33,214	102,151
G19	4637	3536	6745
G20	16,971	12,096	26,892
G21	8147	3162	7442
G22	14,457	7242	18,523
G23	14,525	9671	15,193
G24	3442	1514	3022
6th year			
G01	37,848	41,331	61,292
G02	79,839	25,510	85,563
G03	32,855	16,495	34,354
G04	350,540	236,424	655,308
G05	8370	3602	12,712
G06	46,584	26,398	53,566
G07	16,892	7440	23,587
G08	27,271	9900	35,873
G09	22,653	11,804	42,209
G10	8738	6144	17,186
G11	31,398	20,102	7421
G12	5046	3306	6200
G13	24,887	5190	34,655
G14	18,112	8054	22,085
G15	7765	5879	14,333
G16	43,790	18,939	41,081
G17	22,957	8194	17,907
G18	95,156	40,275	103,366
G19	2589	4284	9986
G20	35,656	15,878	25,662
G21	9399	6479	7364
G22	3437	9150	16,379
G23	17,489	8704	15,883
G24	822	2579	2582
7th year			
G01	70,019	35,348	91,848
G02	92,488	54,416	81,006
G03	20,019	19,429	33,165
G04	269,807	115,749	495,853
G05	10,035	2439	12,378
G06	68,584	29,961	43,254
G07	16,636	8694	20,569
G08	13,324	18,070	40,562
G09	28,148	17,246	20,565
G10	5804	6238	12,888
G11	6039	9934	23,552
G12	6515	2658	5132
G13	41,455	13,421	29,086
G14	21,249	8959	15,008
G15	9197	3320	12,552
G16	59,223	16,115	43,151
G17	13,322	6847	26,592
G18	77,359	35,828	87,655
G19	8435	3104	8679
G20	20,236	8522	12,318
G21	7375	575	12,537
G22	12,843	10,765	14,676
G23	20,815	6128	14,248
G24	5294	1569	3082

Sub-region	White sugar	Raw sugar	Ethanol
8th year			
G01	77,585	22,353	75,116
G02	60,651	35,034	93,484
G03	21,598	12,804	27,094
G04	589,705	136,193	672,791
G05	8060	6638	7869
G06	45,772	29,352	43,579
G07	11,444	5579	18,363
G08	27,791	19,832	28,098
G09	23,466	14,446	41,204
G10	17,446	5687	15,949
G11	32,335	12,262	33,185
G12	10,223	1883	4010
G13	25,940	17,717	39,359
G14	14,105	4675	25,762
G15	12,560	6126	12,283
G16	33,300	26,912	47,714
G17	14,549	10,084	23,989
G18	78,210	35,304	115,779
G19	8305	4328	7250
G20	31,068	15,178	24,256
G21	6422	4269	11,348
G22	28,174	5267	13,268
G23	9430	6776	11,364
G24	1810	1816	2790
9th year			
G01	61,168	43,340	40,564
G02	80,033	41,837	115,077
G03	21,797	12,515	28,055
G04	264,304	200,822	505,320
G05	10,181	6137	486
G06	53,675	30,418	67,046
G07	9534	7554	14,329
G08	31,868	14,063	17,189
G09	30,310	12,046	36,014
G10	12,923	7355	10,558
G11	19,663	16,414	48,901
G12	5303	2316	9022
G13	34,221	10,015	23,035
G14	13,204	14,507	15,897
G15	8287	5250	12,466
G16	37,992	12,695	35,650
G17	27,519	10,949	15,357
G18	57,498	52,188	117,496
G19	7123	4435	10,312
G20	17,120	15,918	28,450
G21	6321	4036	12,418
G22	15,344	4745	19,232
G23	11,604	9085	8667
G24	4371	1855	3400
10th year			
G01	32,748	45,740	106,252
G02	37,934	43,025	101,691
G03	32,081	9455	28,496
G04	262,056	214,018	418,869
G05	10,616	4530	8762
G06	56,416	29,465	36,161
G07	7920	9350	14,600
G08	27,751	17,284	30,577
G09	23,619	22,553	29,771
G10	13,940	8626	13,222
G11	11,035	23,497	28,579
G12	8965	3376	9916
G13	33,963	14,753	20,669
G14	9150	8826	25,143
G15	12,940	7330	11,127
G16	51,390	19,344	44,512
G17	15,441	11,464	5051
G18	94,839	9228	99,030
G19	8863	4993	9382
G20	16,774	13,850	29,062
G21	12,074	6657	6582
G22	16,284	10,906	24,103
G23	10,322	7003	11,422
G24	3657	680	3153

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9.2 Design and planning of infrastructures for bioethanol and sugar production under demand uncertainty

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Design and planning of infrastructures for bioethanol and sugar production under demand uncertainty

A.M. Kostin[a], *G. Guillén-Gosálbez*[a,*], *F.D. Mele*[b], *M.J. Bagajewicz*[c], *L. Jiménez*[a]

[a] *Departament d'Enginyeria Química (EQ), Escola Tècnica Superior d'Enginyeria Química (ETSEQ), Universitat Rovira i Virgili (URV), Campus Sescelades, Avinguda Països Catalans, 26, 43007 Tarragona, Spain*
[b] *Dpto. Ingeniería de Procesos, FACET, Universidad Nacional de Tucumán, Av. Independencia 1800, S. M. de Tucumán T4002BLR, Argentina*
[c] *School of Chemical, Biological and Materials Engineering, University of Oklahoma, Norman, OK 73019, USA*

ABSTRACT

In this paper, we address the strategic planning of integrated bioethanol–sugar supply chains (SC) under uncertainty in the demand. The design task is formulated as a multi-scenario mixed-integer linear programming (MILP) problem that decides on the capacity expansions of the production and storage facilities of the network over time along with the associated planning decisions (i.e., production rates, sales, etc.). The MILP model seeks to optimize the expected performance of the SC under several financial risk mitigation options. This consideration gives a rise to a multi-objective formulation, whose solution is given by a set of network designs that respond in different ways to the actual realization of the demand (the uncertain parameter). The capabilities of our approach are demonstrated through a case study based on the Argentinean sugarcane industry. Results include the investment strategy for the optimal SC configuration along with an analysis of the effect of demand uncertainty on the economic performance of several biofuels SC structures.

Keywords: Supply chain optimization; Planning; Bioethanol supply chain; Sugar supply chain; Financial risk management; Stochastic programming

1. Introduction

Ethanol is nowadays regarded as a successful example of a global shift away from fossil sources of energy to bio-based fuels. The use of ethanol as a transport fuel began in the 1970s, and was motivated by the oil crisis and the need to develop alternative fuel programs for reducing the dependence on oil. Among the various alternative fuels, ethanol is one of the most suitable ones for spark-ignition engines. It is produced from renewable sources and does not contain the impurities present in petroleum-derived products, such as sulphur compounds and carcinogenic aromatics, which are the main sources of pollution in large metropolitan areas. Ethanol and ethanol–gasoline blends have several advantages over conventional gasoline such as the reduction of fossil-originated CO_2 emissions, better anti-knock characteristics, and higher power output and fuel economy (Hsieh et al., 2002). Moreover, the higher auto-ignition temperature and flash point of ethanol lead to lower evaporation loses (Niven, 2005). The use of ethanol has also some disadvantages such as the increase of NO_x and noise emissions (Bayraktar, 2005; Keshkin, 2010). In addition, the gasoline blends with ethanol have a tendency to absorb water and therefore require special storage conditions to prevent a degradation of fuel properties (Muzikova et al., 2009).

Fuel ethanol was firstly adopted by Henry Ford in 1896. The large-scale production of ethanol for the transportation sector, however, did not begin until the late 1970s, and took place mainly in Brazil and US. In 1975, Brazil launched the national alcohol program *Pró-álcool* sponsoring the development of ethanol-fueled cars. By 1986, 72.6% of light vehicles sold in Brazil operated exclusively with pure ethanol (ANFAVEA,

* Corresponding author.
E-mail addresses: andrey.kostin@urv.cat (A.M. Kostin), gonzalo.guillen@urv.cat (G. Guillén-Gosálbez), fmele@herrera.unt.edu.ar (F.D. Mele), bagajewicz@ou.edu (M.J. Bagajewicz), laureano.jimenez@urv.cat (L. Jiménez).
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Nomenclature

Indices

e	scenario
i	material
g	sub-region
k	target value
l	transportation mode
p	manufacturing technology
s	storage technology
t	time period

Sets

$IL(l)$	set of materials that can be transported via transportation mode l
$IM(p)$	set of main products for each technology p
$IS(s)$	set of materials that can be stored via storage technology s
SEP	set of products that can be sold
$SI(i)$	set of storage technologies that can store materials i

Parameters

$\alpha^{PL}_{p,g,t}$	fixed investment coefficient for technology p
$\alpha^{S}_{s,g,t}$	fixed investment coefficient for storage technology s
β	storage period
$\beta^{PL}_{p,g,t}$	variable investment coefficient for technology p
$\beta^{S}_{s,g,t}$	variable investment coefficient for storage technology s
$\rho_{p,i}$	material balance coefficient associated with material i and technology p
τ	minimum desired percentage of the available installed capacity
φ	tax rate
avl_l	availability of transportation mode l
$CapCrop_{g,t}$	total capacity of sugar cane plantations in sub-region g in time t
$DW_{l,t}$	driver wage
$EL_{g,g'}$	distance between g and g'
$\overline{FCI}$	upper limit on the capital investment
FE_l	fuel consumption of transport mode l
$FP_{l,t}$	fuel price
$GE_{l,t}$	general expenses of transportation mode l
$LT_{i,g}$	landfill tax
ME_l	maintenance expenses of transportation mode l
$\overline{PCap_p}$	maximum capacity of technology p
$\underline{PCap_p}$	minimum capacity of technology p
$\overline{PR}_{i,g,t}$	prices of final products
$\overline{Q_l}$	maximum capacity of transportation mode l
$\underline{Q_l}$	minimum capacity of transportation mode l
$\overline{SCap_s}$	maximum capacity of technology p
$\underline{SCap_s}$	minimum capacity of storage technology s
$\overline{SD}_{i,g,t,e}$	demand of product i in sub-region g in time t in scenario e
SP_l	average speed of transportation mode l
sv	salvage value
T	number of time intervals
$TCap_l$	capacity of transportation mode l
$TMC_{l,t}$	cost of establishing transportation mode l in period t
$UPC_{i,p,g,t}$	unit production cost
$USC_{i,s,g,t}$	unit storage cost

Variables

$CF_{t,e}$	cash flow in time t in scenario e
$DC_{t,e}$	disposal cost in time t in scenario e
$DTS_{i,g,t,e}$	amount of material i delivered in sub-region g in period t in scenario e
$FC_{t,e}$	fuel cost in time t in scenario e
FCI	fixed capital investment
$FOC_{t,e}$	facility operating cost in time t in scenario e
$FTDC_{t,e}$	fraction of the total depreciable capital in time t in scenario e
$GC_{t,e}$	general cost in time t in scenario e
$LC_{t,e}$	labor cost in time t in scenario e
$MC_{t,e}$	maintenance cost in time t in scenario e
$NE_{t,e}$	net earnings in time t in scenario e
$NP_{p,g,t}$	number of plants operating with technology p installed in sub-region g in time t
NPV_e	net present value in scenario e
$NS_{s,g,t}$	number of storage facilities of type s established in sub-region g in time t
$NT_{l,t}$	number of transportation units l
$PCap_{p,g,t}$	capacity of technology p in sub-region g in time t
$PCapE_{p,g,t}$	capacity expansion of technology p executed in sub-region g in time t
$Q_{i,l,g,g',t,e}$	flow rate of material i transported by mode l from sub-region g' to sub-region g in time t in scenario e
$Rev_{t,e}$	revenue in time t in scenario e
$SCap_{s,g,t}$	capacity of storage s in sub-region g in time t
$SCapE_{s,g,t}$	capacity expansion of storage s in sub-region g in time t
$ST_{i,s,g,t,e}$	total inventory of material i in sub-region g stored by technology s in time t in scenario e
$TOC_{t,e}$	transport operating cost in time t in scenario e
$PE_{i,p,g,t,e}$	production rate of material i produced by technology p in sub-region g in time t in scenario e
$PT_{i,g,t,e}$	total production rate of material i in sub-region g in time t in scenario e
$PU_{i,g,t,e}$	purchase of material i in sub-region g in time t in scenario e
$X_{l,g,g',t}$	binary variable (1 if a transportation link of type l is established between sub-regions g and g' in period t, and 0 otherwise)
$W_{i,g,t,e}$	amount of waste i generated in sub-region g in time t in scenario e

2009). In 1976, the ethanol–gasoline blend became mandatory in Brazil. Since 2007, this blend should contain at least 25% of ethanol. With this energy policy, the percentage of renewable energy in the Brazilian energy matrix reached 45% in 2006 (Dias Leite, 2009). In 1978, the US Congress approved the Energy Tax Act to promote the usage of renewable energy through taxes and tax credits, and as result, USA overtook Brazil as the biggest ethanol producer in 2005, and by 2009, there were 170 ethanol distilleries with a total annual capacity 10.6 billion of gallons(RFA, 2009).

Vast investments, government sponsorship and tax incentives made Brazil and US the world leaders in ethanol production, currently covering about 90% of the ethanol production worldwide. Other countries have also started to adopt legislation and sponsor bioethanol programs. In 2007, the Argentinean Government published the Law 26,093 on biofuels, which has the target of achieving by 2010 a mix of 5% of ethanol in gasoline and 5% of bio-diesel in diesel. The Colombian Law 693 published in 2001 established a limit of 10% ethanol blend by 2006, and a 25% blend within 15 years. In Thailand, the goal is to achieve a 10% ethanol blend by 2011. In India, the Indian Ethanol Blended Petrol (EBP) program specifies a target of 5% ethanol gasoline blends. Canada also started to provided tax benefits for ethanol producers and consumers in 1992. The EU is no exception to this general trend, having established quantitative targets for the use of biofuels. Particularly, by 2010, it plans to replace 5.75% of diesel and gasoline by biofuels (Olsson, 2007).

The adoption of alternative energy sources has recently created a clear need for decision-support tools to assist in the design of infrastructures for biofuels production from biomass. Among the available methods, those based on mathematical programming have gained wider interest in the recent past. The main advantage of these tools is their capability of generating and assessing a very large number of process alternatives, from which the optimal one is selected. The prevalent approaches in this area have relied on linear programming (LP) and mixed-integer linear programming (MILP).

Several models have been proposed for optimizing bioethanol SCs. Yoshizaki et al. (1996) introduced an LP model to find the optimal distribution of sugarcane mills, fuel bases and consumer cites in southeastern Brazil. Kawamura et al. (2006) presented an LP model to minimize the transportation and external storage costs of the existing sugar/ethanol SC in Brazil. Ioannou (2005) applied an LP optimization model to reduce the transportation cost in the Greek sugar industry. The MILP model of Milan et al. (2006) minimizes the transportation cost of the sugarcane SC in Cuba. Dunnett et al. (2008) developed a combined production and logistic model to find the optimal configuration of lignocellulosic bioethanol SCs. Zamboni et al. (2009) presented a mathematical model to minimize the total daily 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. (2007), Paiva and Morabito (2009), Colin (2009) and Higgins and Laredo (2006).

The environmental assessment of bioethanol production has gained wider interest in the recent past. Several models have been presented so far to optimize simultaneously the economic and environmental performance of bioethanol SCs. These approaches have mainly focused on reducing the greenhouse gas (GHG) emissions of the biofuel infrastructure. Zamboni et al. (2009) formulated a multi-objective optimization model to reduce the GHG emissions associated with the future corn-based Italian bioethanol network. Later, Giarola et al. (2011) extended this model by adding second generation bioethanol production technologies. It has been argued that minimizing exclusively the GHGs emission in the design of ethanol infrastructures can lead to solutions that reduce such emissions at the expense of increasing other negative effects (mainly the destruction of the native tropical ecosystems and soil erosion) (Scharlemann and Laurance, 2008; Vries et al., 2010). To overcome this limitation, Mele et al. (2011) developed a bi-criteria model that maximizes the profit and minimizes the life cycle environmental impact of combined sugar/bioethanol SCs. The latter criterion was measured through two environmental indicators: the eco-indicator 99 (Goedkoop and Spriensma, 1999), which accounts for eleven life cycle environmental impacts pertaining to several damage categories, and the global warming potential.

The studies mentioned above assume that all model parameters are perfectly known in advance (i.e., they are constant). In practice, however, some of them, especially the demand, show certain degree of variability and can therefore be regarded as uncertain. Various approaches have been proposed to formulate and solve optimization models with uncertain parameters (see Sahinidis, 2004). Particularly, two-stage stochastic programming is probably the prevalent approach to deal with optimization under uncertainty (Liu and Sahinidis, 1996). Two-stage stochastic formulations involve two types of decisions: first stage decisions that must be made before the realization of the uncertain parameters, and second stage decisions that are taken once the uncertainty is unveiled. The goal is to choose the first-stage variables in a way that the expected value of the objective function is maximized or minimized over all the scenarios. Robust optimization is an alternative approach to handle uncertainties that relies on the use of chance-constraints. Following this approach, the original robust stochastic model is typically substituted by a deterministic formulation with several equations representing the probabilistic statements expressed through chance constraints (Li et al., 2008). The main drawback of this technique is that it does not include second-stage variables, that is, it does not quantify the effect of each uncertain outcome when it materializes. Fuzzy programming (Zimmermann, 1991) is another approach to deal with uncertainties that relies on modeling the random parameters as fuzzy numbers and treating the model constraints as fuzzy sets.

To the best of our knowledge, there are only two works in the literature that have accounted for uncertainties in the optimization of biofuel infrastructures. Dal-Mas et al. (2011) proposed a scenario-based MILP model that maximizes the expected profit and minimizes the financial risk of the corn-to-ethanol production SC in Northern Italy. The model takes into account the uncertainty of the corn purchase cost and ethanol selling price. Kim et al. (2011) presented a two-stage MILP model for optimizing a bio-oil network in the SE region of the US under uncertainty in 14 key model parameters. The authors performed also a sensitivity analysis to estimate key factors affecting the SC performance.

This article introduces a novel two stage MILP formulation for the strategic planning of SCs for bioethanol and sugar production under demand uncertainty. To the best of our knowledge, this is the first contribution that addresses explicitly the uncertainty associated with the bioethanol and sugar demand and analyzes its impact on the optimal SC structure and economic performance of the network considering several risk metrics. A decomposition strategy based on the sample average approximation (SAA) (Verweij et al., 2003) algorithm is also presented to efficiently solve the underlying stochastic MILP. This algorithm provides as output a set of SC design alternatives that behave in different ways in the face of uncertainty.

The remainder of this article is organized as follows. In Section 2, the problem under study is formally stated, and

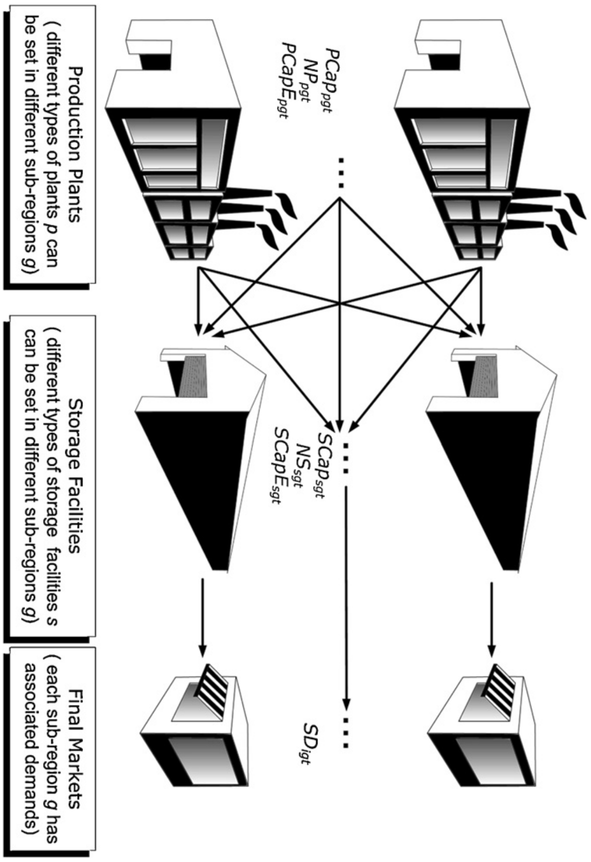

Fig. 1 – Structure of the bioethanol/sugar SC.

the assumptions made are briefly described. The problem data, decision variables and objectives are also listed at this point. In Section 3, we describe a two-stage stochastic model for the design and planning of bioethanol SCs that considers explicitly the demand variability. In Section 4, we introduce a decomposition method based on the SAA algorithm that provides approximate solutions to the multi-objective stochastic formulation in short CPU times. In Section 5, the proposed approach is applied to a real case study based on the sugarcane industry of Argentina, for which valuable insights are obtained. The conclusions of the work are finally drawn in the last section of the paper.

2. Problem statement

Fig. 1 depicts the SC structure we use in our work. We analyze integrated infrastructures for the combined production of ethanol and sugar, in which final products (ethanol, white and raw sugars) are stored in warehouses before being delivered to the final markets. Two different types of storage facilities are considered that are suitable for solid (S1) and liquid (S2) materials, respectively. The SC facilities can be located in different sub-regions, and are connected via transportation links. We consider three types of vehicles: heavy trucks for sugarcane (TR1), lorries for sugars (TR2), and tank trucks for ethanol and all types of vinasse (TR3).

The problem addressed in this article can be formally stated as follows. Given are a set of potential locations for the SC facilities, the capacity limitations associated with these technologies, the demand and prices of final products and raw materials and the investment and operating cost of the network. The demand is assumed to be uncertain, and it is described through a set of scenarios with a given probability of occurrence. The goal of the study is to determine the configuration of the SC along with the associated planning decisions that maximize its economic performance under uncertainty.

3. Stochastic mathematical model

3.1. General features

The general structure of the mathematical model presented next is based on previous works by the authors (see Guillén-Gosálbez and Grossmann, 2009 and Guillén-Gosálbez et al., 2009). Our model has been originally devised bearing in mind the main features of the sugarcane industry of Argentina, but it is general enough to be easily extended to any other supply chain with similar characteristics.

Argentina has abundant natural resources and an efficient agricultural sector (Ken and Wilder, 2010). Sugarcane, in particular, shows several appealing characteristics compared to other products, such as its resistance, rapid growth and uptake capacity for atmospheric carbon. This makes sugarcane a suitable feedstock for biofuels production. The main advantage of the production of ethanol from sugarcane is its positive energy balance (Goldemberg et al., 2008). Unfortunately, the use of ethanol in Argentina has the disadvantage of competing with sugar, because both of them share the same raw material. A key issue in the optimization of bioethanol infrastructures in Argentina is then the assessment of the interactions between both competing products.

The following assumptions, some of which are based on the particular features of the Argentinean sugarcane industry, are applied in the derivation of our model:

Production. It is assumed that the juice is extracted from sugarcane mainly by milling. Sugar mills use this juice to produce white sugar and raw sugar. There are two technologies that follow the "sugarcane-to-sugar" pathway. One of them generates molasses (T1) as a byproduct, whereas the other one produces a secondary honey (T2) in addition to sugars. These two byproducts differ in their sucrose content. Molasses is a viscous dark honey whose low sucrose content cannot be separated by crystallization, while the secondary honey is a honey with a larger amount of sucrose that leaves the sugar mill before being exhausted by crystallization. Anhydrous ethanol can be produced by fermentation and subsequent dehydration of different process streams: molasses (T3), honey (T4), and sugarcane juice (T5). Thus, the model considers a total of five different technologies, two for sugar production and three types of distilleries. The details of each technology, including the mass balance coefficients, are shown in Fig. 2, where residuals, loses and wastes are omitted. We assume that the bagasse is completely utilized for internal purposes, so there is a total of nine materials classified into raw materials, byproducts, and final products: sugarcane, ethanol, molasses, honey, white sugar, raw sugar, vinasse type 1, vinasse type 2 and vinasse type 3. Each plant incurs fixed capital and operating cost, and can be expanded in capacity over time in order to follow a specific demand pattern.

Storage. The model includes two different types of storage facilities: warehouses for liquid products (S1), and warehouses for solid materials (S2). For each storage facility type, we consider specific fixed capital and unit storage costs, along with

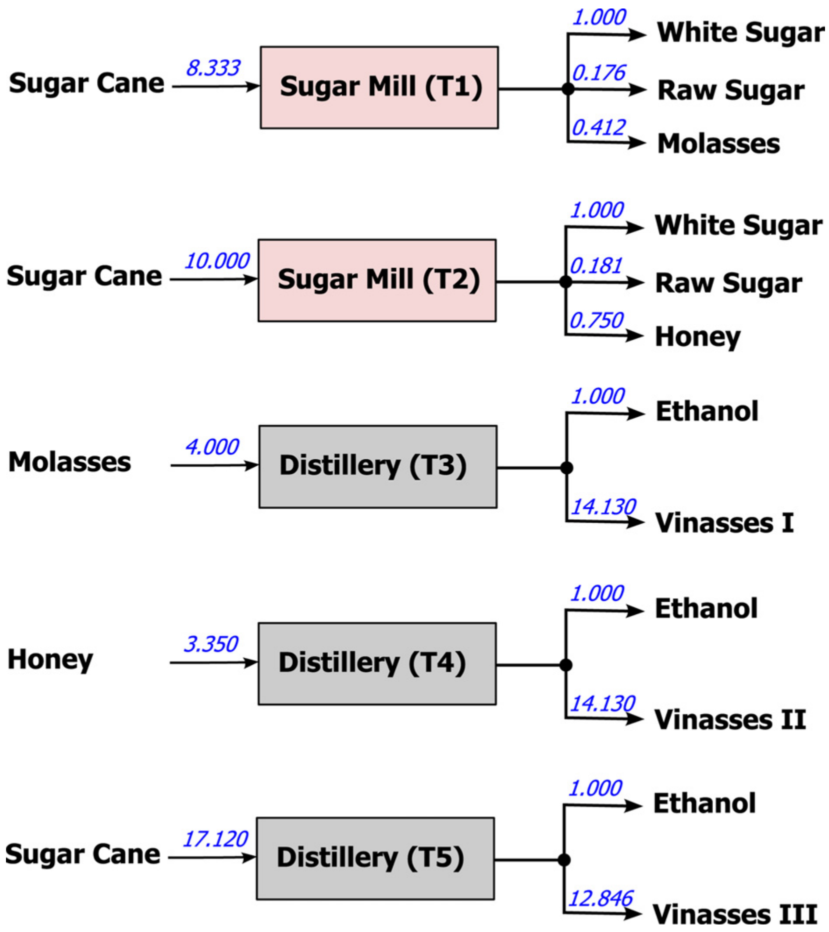

Fig. 2 – Set of production technologies.

lower and upper limits on its capacity expansions. Similarly, as with the plants, 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 the customers, supply the production plants with raw materials, and dispose the process wastes. The model assumes that the materials can be transported by three different types of trucks: heavy trucks with open-box bed for sugar cane (TR1), medium trucks for sugar (TR2), and tank trucks for liquid products (TR3). Each transportation mode has fixed capital and unit transportation costs, and lower and upper limits on its capacity. Both storage and transportation modes considered in the model are shown in Fig. 3.

3.2. *Model structure: two-stage stochastic programming*

A number of deterministic models have been published to model and optimize the structure of SCs (Chen and Wang, 1997; Timpe and Kallrath, 2000; Bok et al., 2000; Almansoori and Shah, 2006). These models assume that all model parameters are perfectly known in advance and do not show variability. In practice, however, there are numerous technical and market uncertainties that affect the calculations. One of the most important sources of uncertainty in any SC is the product demand. Failure to properly account for product demand fluctuations may result in either unsatisfied customer demand or excess of products. The first scenario leads to a loss of potential revenues and market share, whereas the second one generates large inventory costs.

We introduce next a two-stage stochastic programming MILP model to address the strategic planning of biofuels SCs under demand uncertainty. The equations of the model are roughly classified into three main blocks: mass balance equations, capacity constraints and objective function equations. With regard to the variables, these are divided into two main groups:

- *First-stage*, or *here-and-now* decisions, which are taken before the uncertainty unveils. In our work, the SC design decisions, namely the number of production, storage and transportation units, and their initial capacities and capacity expansions over the time horizon are considered as first stage decisions. The reason for this is that we assume that they are taken at the beginning of the time horizon, before the demand is known.
- *Second-stage*, or *wait-and-see* decisions, which are taken once the uncertainty is materialized. They include the amount of products to be produced and stored, the flows of materials transported among the SC entities and the product sales. As will be shown later in the article, the second-stage variables include a subscript *e* that denotes the particular scenario realization for which they are defined.

The sections that follow describe in detail all the variables and constraints of the model.

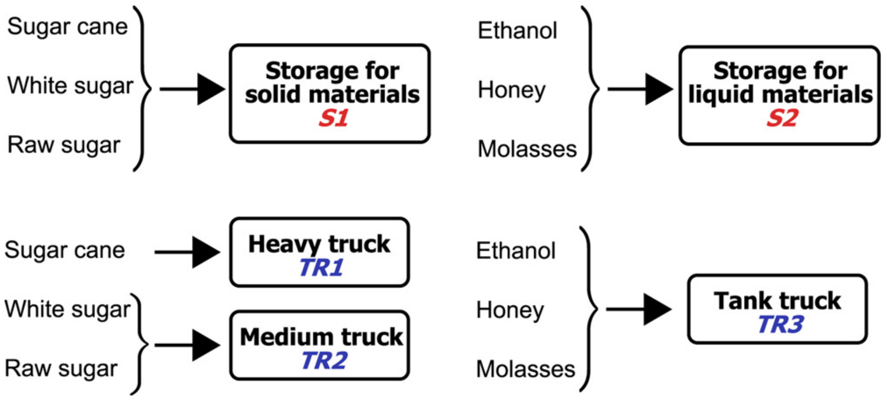

Fig. 3 – Set of storage and transportation technologies.

3.3. *Mass balance constraints*

The overall mass balance for each sub-region is enforced via Eq. (1). For every material form i and scenario e, the initial inventory kept in sub-region g ($ST_{i,s,g,t-1,e}$) plus the amount produced ($PT_{i,g,t,e}$), the amount of raw materials purchased ($PU_{i,g,t,e}$) and the input flow rate from other facilities in the SC ($Q_{i,l,g',g,t,e}$) must equal the final inventory ($ST_{i,s,g,t,e}$) plus the amount delivered to the customers ($DTS_{i,g,t,e}$) plus the output flow to other facilities in the SC ($Q_{i,l,g,g',t,e}$) and the amount of waste ($W_{i,g,t,e}$).

$$\sum_{s\in SI(i)} ST_{i,s,g,t-1,e} + PT_{i,g,t,e} + PU_{i,g,t} + \sum_{l\in LI(i)} \sum_{g' \neq g} Q_{i,l,g',g,t,e} = \sum_{s\in SI(i)} ST_{i,s,g,t,e} + DTS_{i,g,t,e} + \sum_{l\in LI(i)} \sum_{g' \neq g} Q_{i,l,g,g',t,e} + W_{i,g,t,e} \quad \forall i, g, t, e \tag{1}$$

In this equation, $SI(i)$ represents the set of technologies that can be used to store product i, whereas $LI(i)$ is the set of transport modes suitable for product i.

For each scenario e, the total production rate of material i in sub-region g is determined from the production rates associated with each technology p installed in that sub-region ($PE_{i,p,g,t,e}$):

$$PT_{i,g,t,e} = \sum_{p} PE_{i,p,g,t,e} \quad \forall i, g, t, e \tag{2}$$

The production rates of byproducts and the consumption rates of raw materials associated with each technology are calculated in each scenario e from the material balance coefficient ρ_{pi}, and the production rate of the main product:

$$PE_{i,p,g,t,e} = \rho_{p,i} PE_{i\prime,p,g,t,e} \quad \forall i, p, g, t, e \quad \forall i\prime \in IM(p) \tag{3}$$

In this equation, $IM(p)$ represents the set of main products associated with each technology. Fig. 2 shows the material balance coefficients of the main products (white sugar and ethanol). Note that these parameters are typically normalized to 1.

For each scenario e and time interval t, the purchases of sugarcane are limited by the capacity of the existing sugarcane plantation in sub-region g:

$$PU_{i,g,t,e} \leq CapCrop_{g,t} \quad i = \text{Sugarcane}, \forall g, t, e \tag{4}$$

The total inventory of product i stored at the end of the time interval t in each scenario e ($ST_{i,s,g,t,e}$) must be less than or equal to the available storage capacity ($SCap_{s,g,t}$):

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

The average inventory in scenario e ($AIL_{i,g,t,e}$) is a function of the amount delivered to the customers and the storage period β:

$$AIL_{i,g,t,e} = \beta DTS_{i,g,t,e} \quad \forall i, g, t, e \tag{6}$$

The storage capacity ($SCap_{s,g,t}$) that should be established in a sub-region in order to cope with fluctuations in both supply and demand, is twice the summation of the average inventory levels of products i (Simchi-Levi et al., 2000) in each scenario e:

$$2AIL_{i,g,t,e} \leq \sum_{s\in SI(i)} SCap_{s,g,t} \quad \forall i, g, t, e \tag{7}$$

Furthermore, the amount of product i delivered to the final markets located in region g in scenario e and period t should be less than or equal to the corresponding demand in that region ($SD_{i,g,t,e}$):

$$DTS_{i,g,t,e} \leq SD_{i,g,t,e} \quad \forall i, g, t, e \tag{8}$$

3.4. *Capacity constraints*

The production rate of each technology p in sub-region g and scenario e must lie between the minimum desired percentage of the available technology that must be utilized, τ, multiplied by the existing capacity (represented by the continuous variable $PCap_{p,g,t}$) and the maximum capacity:

$$\tau PCap_{p,g,t} \leq PE_{i,p,g,t,e} \leq PCap_{p,g,t} \quad \forall i, p, g, t, e \tag{9}$$

The capacity of technology p in any time period t is calculated from the existing capacity at the end of the previous period and the expansion in capacity, $PCapE_{p,g,t}$, carried out in period t:

$$PCap_{p,g,t} = PCap_{p,g,t-1} + PCapE_{p,g,t} \quad \forall p, g, t \tag{10}$$

Eq.(11) limits the capacity expansion $PCapE_{p,g,t}$ between upper and lower bounds, which are calculated from the number of plants installed in the sub-region ($NP_{g,p,t}$) and the minimum and maximum capacity associated with each technology p ($\underline{PCap_p}$ and $\overline{PCap_p}$, respectively).

$$\underline{PCap_p} NP_{p,g,t} \le PCapE_{p,g,t} \le \overline{PCap_p} NP_{p,g,t} \quad \forall p, g, t \tag{11}$$

The storage capacity must lie within certain lower and upper bounds that are calculated from the number of storage facilities installed in sub-region g ($NS_{s,g,t}$) and the minimum and maximum storage capacities ($\underline{SCap_s}$ and $\overline{SCap_s}$, respectively) associated with each storage technology:

$$\underline{SCap_s} NS_{s,g,t} \le SCapE_{s,g,t} \le \overline{SCap_s} NS_{s,g,t} \quad \forall s, g, t \tag{12}$$

The capacity of a storage technology s in region g and 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 ($SCapE_{s,g,t}$):

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

The materials flows in scenario e are constrained within some minimum and maximum allowable capacity limits ($\underline{Q_l}$ and $\overline{Q_l}$, respectively):

$$\underline{Q_l} X_{l,g,g',t} \le \sum_{i \in IL(l)} Q_{i,l,g,g',t,e} \le \overline{Q_l} X_{l,g,g',t} \quad \forall l, t, g, g'(g' \ne g), e \tag{14}$$

In this equation, $IL(l)$ represents the set of materials that can be transported via transportation mode l.

3.5. *Objective function*

The model shows a different economic performance in each scenario. In our case, this economic performance is measured through the net present value (NPV). Thus, one objective of the mathematical formulation is to maximize the expected value of the resulting NPV distribution. Certain risk metrics are also appended to the objective function in order to control the probability of unfavorable scenarios with low NPV values. The sections that follows describe how these metrics are determined.

3.5.1. *Expected NPV*

One of the objectives of the model is to maximize the expected NPV. This metric is determined as follows:

$$E[NPV] = \sum_e pr_e NPV_e \tag{15}$$

where pr_e is the probability of scenario e, and NPV_e is the net present value attained in the same scenario. The latter term is determined from the cash flows ($CF_{t,e}$) generated in each of the time intervals t in which the total time horizon is divided:

$$NPV_e = \sum_t \frac{CF_{t,e}}{(1+ir)^{t-1}} \quad \forall e \tag{16}$$

In this equation, ir represents the interest rate. The cash flow in period t is determined from the net earnings $NE_{t,e}$ (i.e., profit after taxes), and the fraction of the total depreciable capital ($FTDC_t$) that corresponds to that period as follows:

$$CF_{t,e} = NE_{t,e} - FTDC_t \quad t = 1, \ldots, T-1, \forall e \tag{17}$$

When determining the cash flow of the last time period ($t = T$), we consider that part of the total fixed capital investment (FCI) will 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.

$$CF_{t,e} = NE_{t,e} - FTDC_t + svFCI \quad t = T, \forall e \tag{18}$$

The net earnings are given by the difference between the incomes ($Rev_{t,e}$) and the facility operating ($FOC_{t,e}$), and transportation cost ($TOC_{t,e}$), as stated in Eq.(19):

$$NE_{t,e} = (1-\varphi)(Rev_{t,e} - FOC_{t,e} - TOC_{t,e}) + \varphi DEP_{t,e} \quad \forall t, e \tag{19}$$

In this equation, φ denotes the tax rate. The depreciation term is calculated with the straight-line method:

$$DEP_t = \frac{(1-sv)FCI}{T} \quad \forall t \tag{20}$$

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

$$\begin{aligned} FCI = & \sum_p \sum_g \sum_t (\alpha^{PL}_{p,g,t} NP_{p,g,t} + \beta^{PL}_{p,g,t} PCapE_{p,g,t}) \\ & + \sum_s \sum_g \sum_t (\alpha^{S}_{s,g,t} NS_{s,g,t} + \beta^{S}_{s,g,t} SCapE_{s,g,t}) \\ & + \sum_l \sum_t (NT_{l,t} TMC_{l,t}) \end{aligned} \tag{21}$$

Here, the parameters $\alpha^{PL}_{p,g,t}$, $\beta^{PL}_{p,g,t}$ and α^{S}_{sgt}, β^{S}_{sgt} are the fixed and variable investment terms associated with plants and warehouses, respectively. On the other hand, $TMC_{l,t}$ is the purchase cost associated with the transportation mode l. The average number of trucks required to satisfy a certain flow between different sub-regions is calculated from the flow rate of products between the sub-regions, the transportation mode availability (avl_l), the capacity of a transport container, the average distance traveled between the sub-regions, the average speed, and the loading/unloading time, as stated in Eq. (22):

$$\sum_{t \le T} NT_{l,t} = \sum_{i \in IL(l)} \sum_g \sum_{g' \ne g} \sum_t \frac{Q_{i,l,g,g',t}}{avl_l TCap_l} \left(\frac{2EL_{g,g'}}{SP_l} + LUT_l \right) \quad \forall l \tag{22}$$

The revenues are determined from the sales of final products and the corresponding prices ($PR_{i,g,t}$):

$$Rev_{t,e} = \sum_{i \in SEP} \sum_{g} DTS_{i,g,t,e} PR_{i,g,t} \quad \forall t, e \tag{23}$$

In this equation, $SEP(i)$ represents the set of materials i that can be sold. The facility operating cost is obtained by multiplying the unit production and storage costs ($UPC_{i,p,g,t}$ and $USC_{i,s,g,t}$, respectively) with the corresponding production rates and average inventory levels, respectively. This term includes also the disposal cost ($DC_{t,e}$):

$$FOC_{t,e} = \sum_{i \in IM(p)} \sum_{p} \sum_{g} UPC_{i,p,g,t} PE_{i,p,g,t,e} + \sum_{i \in IS(s)} \sum_{s} \sum_{g} USC_{i,s,g,t} AIL_{i,g,t,e} + DC_{t,e} \quad \forall t, e \tag{24}$$

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

$$DC_{t,e} = \sum_{i} \sum_{g} W_{i,g,t,e} LT_{ig} \quad \forall t, e \tag{25}$$

The transportation cost includes the fuel ($FC_{t,e}$), labor ($LC_{t,e}$), maintenance ($MC_{t,e}$) and general ($GC_{t,e}$) costs:

$$TOC_{t,e} = FC_{t,e} + LC_{t,e} + MC_{t,e} + GC_{t,e} \quad \forall t, e \tag{26}$$

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

$$FC_{t,e} = \sum_{i \in IL(l)} \sum_{g} \sum_{g' \neq g} \sum_{l} \left[\frac{2EL_{g,g'} Q_{i,l,g,g',t,e}}{FE_l TCap_l} \right] FP_{l,t} \quad \forall t, e \tag{27}$$

In Eq. (27), the fractional term represents the fuel usage, which is determined from the total distance traveled in a trip ($2EL_{g,g'}$), the fuel consumption of transport mode l (FE_l) and the number of trips made per time period ($Q_{i,l,g,g',t,e}/TCap_l$). This equation considers that the transportation units operate only between two predefined sub-regions. Furthermore, as shown in Eq. (28), the labor transportation cost is a function of the driver wage ($DW_{l,t}$) and total delivery time (term inside the brackets):

$$LC_{t,e} = \sum_{i \in IL(l)} \sum_{g} \sum_{g' \neq g} \sum_{l} DW_{l,t} \left[\frac{Q_{i,l,g,g',t,e}}{TCap_l} \left(\frac{2EL_{g,g'}}{SP_l} + LUT_l \right) \right] \times \forall t, e \tag{28}$$

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

$$MC_{t,e} = \sum_{i \in IL(l)} \sum_{g} \sum_{g' \neq g} \sum_{l} ME_l \frac{2EL_{g,g'} Q_{i,l,g,g',t,e}}{TCap_l} \quad \forall t, e \tag{29}$$

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

$$GC_t = \sum_{l} \sum_{t' \leq t} GE_{lt} NT_{lt'} \quad \forall t \tag{30}$$

The total capital investment can be constrained to be lower than an upper limit, as stated in Eq. (31):

$$FCI \leq \overline{FCI} \tag{31}$$

The model assumes that the depreciation is linear over the time horizon, so the amount of capital investment paid in each time period ($FTDC_t$) is calculated as follows:

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

While NPV has been thoroughly used in several SC designs, caution ought to be exercised. In fact, as pointed out by Bagajewicz (2008), maximizing NPV without control of the capital to invest can lead to solutions that have marginal profit far inferior in terms of return of investment (ROI), which is an alternative objective that one could use. In our case, to overcome this limitation, we limit the FCI.

3.6. *Probabilistic metrics for financial risk management*

The variability of the objective function can be controlled by adding to the model a set of constraints that measure the probability of not attaining a predefined target value Ω. The calculation of these probabilities requires the definition of the binary variable Z_e. This variable takes the value of 1 if the NPV attained in scenario e is below the target level Ω, and it is 0 otherwise. The definition of such a variable is enforced via the following constraints:

$$NPV_e \leq \Omega + M(1 - Z_e) \quad \forall e \tag{33}$$

$$NPV_e \geq \Omega - MZ_e \quad \forall e \tag{34}$$

These equations work as follows. If the binary variable takes a value of 1, then constraint Eq. (33) will force the NPV to be lower than the target value in scenario e, whereas constraint Eq. (34) will be inactive. If the binary variable is 0, then Eq. (33) will be inactive and constraint Eq. (34) will ensure that the NPV in that particular scenario lies above the target value. The probability of having an NPV below Ω is calculated as follows:

$$Prob[NPV \leq \Omega_k] = \sum_{e} pr_e Z_{k,e} \tag{35}$$

where pr_e denotes the probability of scenario e. An example of the definition of these probabilistic metrics in a particular stochastic problem is given in Fig. 4. This figure depicts the cumulative probability curve associated with a given SC design, considering a stochastic formulation with 100 scenarios, each one corresponding to a different materialization of the uncertain parameter (i.e., the demand). Assume that the target Ω is equal to US$350 million. For this particular SC structure, there are 14 scenarios out of 100 with an NPV below this

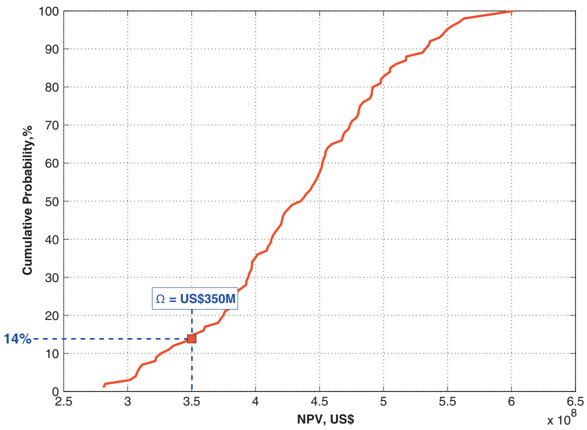

Fig. 4 – Cumulative probability curves.

target value (i.e., the probability of not exceeding the target value is 14%).

In general, the shape and slope of this cumulative probability curve can be manipulated according to the decision-maker's preferences. This can be done by properly adjusting the decisions associated with the SC design and operation. Fig. 5 depicts two cumulative probability curves associated with two different SC topologies. Design A shows lower probabilities of small and high *NPV*s, which would make it appealing for risk-averse decision-makers. On the other hand, design B might be the preferred alternative for risk-takers decision-makers, as it leads to larger probabilities of high *NPV*s at the expense of increasing as well the probability of low benefits.

A widely used risk metric is the value at risk (*VaR*) that can be defined as the difference between E[*NPV*] and the *NPV* value corresponding to a certain level of risk. In this study, this level is set to 5%. The symmetrically opposite measure of risk is the opportunity value (*OV*) (discussed by Aseeri and Bagajewicz, 2004), or upside potential that corresponds to the difference between the *NPV* at 95% risk and the expected value of *NPV*. Fig. 5 presents the calculation of *VaR* and *OV* for the aforementioned risk-averse and risk-taker cumulative probability curves.

The main disadvantage of both *VaR* and *OV* measures is that they cannot represent the behavior of the entire risk curve.

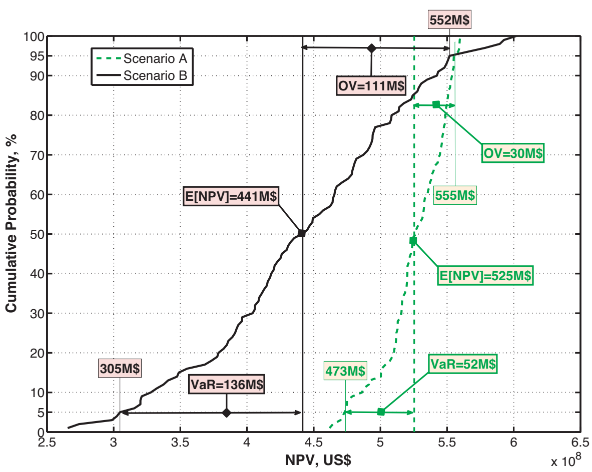

Fig. 5 – Value at risk (VaR) vs. opportunity value (OV).

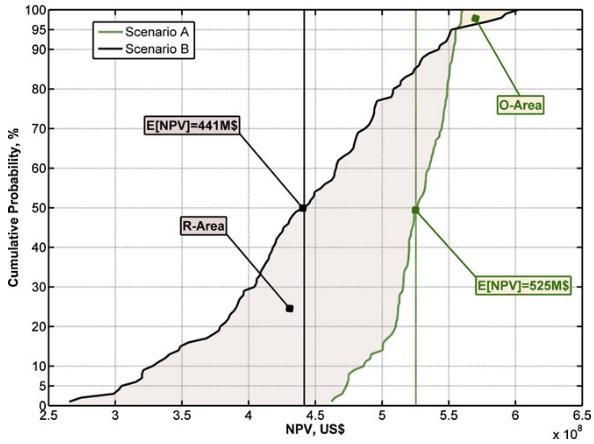

Fig. 6 – Risk area ratio (RAR).

Aseeri and Bagajewicz (2004) also proposed the use of the risk area ratio (*RAR*), which compares the areas between the risk curves corresponding to the reference plan with better E[*NPV*] and the alternative plan being evaluated. The proposed metric is the ratio of the opportunity area (O-Area) enclosed by the two curves above their intersection, to the risk area (R-Area) enclosed by the two curves below their intersection (see Fig. 6). The *RAR* is therefore mathematically defined as follows:

$$RAR = \frac{O-Area}{R-Area} \quad (36)$$

Aseeri and Bagajewicz (2004) claim that a good risk-reduced plan is one with a *RAR* as close to 1 as possible. Rather than solving a multi-objective model that seeks to optimize the aforementioned risk metrics, we propose herein to apply a method based on the sample average approximation algorithm (Verweij et al., 2003; Aseeri and Bagajewicz, 2004; Barbaro and Bagajewicz, 2004). As will be shown later in the article, our approach allows for the identification of SC configurations with different economic performance (measured according to the risk metrics mentioned above) in the face of uncertainty. From these alternatives, decision-makers should choose the best one according to their preferences. The method is described in detail in the following section.

4. Solution method: sample average approximation

The algorithm used to approximate the solution of the stochastic problem entails the calculation of two models that are solved in an iterative manner. A reduced-space stochastic model defined for only one scenario is solved in first place. This provides the values of the strategic and planning decision variables of the problem for that particular scenario. The original stochastic problem (with all the scenarios included) is then solved maximizing the expected *NPV* and fixing the first stage variables to the values provided by the reduced-space stochastic model. Hence, for each set of design variables corresponding to the solution of the reduced-space stochastic model defined for a specific scenario, we construct a risk curve. This procedure is repeated until there are no more scenarios to be explored.

After solving the reduced-space stochastic model for all the scenarios, we obtain a set of risk curves that are next filtered in

Table 1 – Expected demand, ton/year.

Sub-region	Product form		
	White sugar	Raw sugar	Ethanol
Córdoba	84,126	42,063	92,539
Mesopotamia	84,126	42,063	92,539
Buenos Aires	455,884	227,942	501,472
Cuyo	72,108	36,054	79,319
North	39,960	19,980	43,956
North West	47,872	23,936	52,659
Tucumán	37,156	18,578	40,871
Santa Fe	81,122	40,561	89,234
La Pampa	8,413	4,206	9,254
Santiago	21,733	10,866	23,906
West	18,327	9,164	20,160
Patagonia	49,174	24,587	54,091

order to discard those that are dominated by at least another one. One solution A is dominated by another solution B if its probability curve lies entirely above that of B. Note that this implies that for any probability level, A will always lead to lower benefits than B. In other words, A will be better considering the whole range of probability levels. From the set of non-dominated solutions, decision-makers should choose the one that better fits his/her preferences.

The detailed steps of the algorithm are as follows:

1. Set counter *ctr* equal to 1.
2. Solve the stochastic model defined for the scenario whose ordinality is equal to *ctr*.
3. Fix the first stage variables, and solve the stochastic model with all the scenarios included maximizing the expected *NPV*.
4. If $ctr = |E|$ then go to step 5, otherwise make $ctr = ctr + 1$ and go to step 2.
5. Filter the probability curves of the solutions obtained so far by removing the curves dominated by at least another one.
6. End.

Note that the algorithm presented above has been used successfully in a variety of applications to address optimization problems under uncertainty (Whitnack et al., 2009; Lakkhanawat and Bagajewicz, 2008; Lavaja et al., 2006; Pongsakdi et al., 2006; Lavaja and Bagajewicz, 2005, 2004; Guillén-Gosálbez et al., 2005, 2005, 2003; Aseeri et al., 2004; Barbaro and Bagajewicz, 2004; Bonfill et al., 2004; Romero et al., 2003; Bagajewicz and Barbaro, 2003; Koppol and Bagajewicz, 2003; Mele et al., 2003).

5. Case study

We illustrate the capabilities of the proposed approach through a case study based on the sugarcane industry of Argentina. The problem considers 12 sub-regions each one with an associated demand of sugar and ethanol. We should clarify that Argentina is in fact divided into 24 political provinces, some of which have been merged to simplify the calculations. The sub-region "Mesopotamia" comprises the provinces of Corrientes, Misiones and Entre Ríos. The province of Buenos Aires and Buenos Aires city have been merged into the sub-region "Buenos Aires". The sub-region "Cuyo" includes the provinces of Mendoza, San Luis and San Juan. The sub-region "Patagonia" includes the 5 southernmost

Table 2 – Distances between sub-regions, km.

	Córdoba	Mesopotamia	Buenos Aires	Cuyo	North	North West	Tucumán	Santa Fe	La Pampa	Santiago	West	Patagonia
Córdoba	0	900	768	680	880	844	552	340	618	439	433	1196
Mesopotamia	900	0	990	1490	20	830	794	540	1388	635	857	1774
Buenos Aires	768	990	0	1137	1010	1599	1286	541	664	1127	1173	924
Cuyo	680	1490	1137	0	1470	1311	1001	930	789	1007	725	1342
North	880	20	1010	1470	0	810	774	540	1368	618	820	1756
North West	844	830	1599	1311	810	0	310	1077	1462	472	533	2066
Tucumán	552	794	1286	1001	774	310	0	764	1170	159	221	1765
Santa Fe	340	540	541	930	540	1077	764	0	828	605	777	1218
La Pampa	618	1388	664	789	1368	1462	1170	828	0	1050	1065	580
Santiago	439	635	1127	1007	618	472	159	605	1050	0	234	1634
West	433	857	1173	725	820	533	221	777	1065	234	0	1645
Patagonia	1196	1774	924	1342	1756	2066	1765	1218	580	1634	1645	0

Table 3 – Sugarcane capacity, ton/year.

Sub-region	Capacity
Mesopotamia	62,040
North West	6,392,000
Tucumán	12,220,000
Santa Fe	125,960

provinces of Neuquén, Río Negro, Chubut, Santa Cruz and Tierra del Fuego. The provinces of Chaco and Formosa are merged in the sub-region "North", whereas Jujuy and Salta are included in the region "North West". The sub-region "West" includes the provinces of Catamarca and La Rioja. The remaining sub-regions correspond to the homonymous Argentinean provinces.

All these sub-regions along with the mean values of the associated demand are shown in Table 1. The entire set of demand values is provided as supplementary material. The prices for white sugar, raw sugar and ethanol are equal to US$537/ton, US$375/ton and US$860/ton, respectively. Distances between regions have been determined considering the capitals of the corresponding provinces and the main roads connecting them. These data are listed in Table 2. We assume that each region has an associated sugarcane crop capacity. Particularly, sugarcane plantations are situated in only five Argentinean provinces, whose production capacities are represented in Table 3. The length of the planning horizon is equal to 3 years.

The upper bound on the capital investment is US$1.5 billion. The minimum and maximum production capacities of each technology are listed in Table 4. The minimum and maximum storage capacities for liquid and solid materials are assumed to be 50 and 2 billion tons, respectively. Fixed and variable investment coefficients for different production and storage modes are listed in Tables 5 and 6, respectively. Unit production cost for sugar and ethanol are equal to US$265/ton and US$317/ton, respectively. The unit storage cost is US$0.365/(ton·year) for all types of materials. The parameters used to calculate the capital and operating cost for different transportation modes can be found in Table 7. The minimum flow rate of each transportation mode is assumed to be equal to the minimum capacity of the corresponding transportation mode, whereas the maximum flow rates for heavy trucks, medium trucks and tanker trucks are 6.25, 6.25 and 6.00 million tons per year, respectively.

The stochastic model with 100 scenarios was written in GAMS (Rosenthal, 2008) and solved with the MILP solver CPLEX 11.0 on a HP Compaq DC5850 desktop PC with an AMD Phenom 8600B, 2.29 GHz triple-core processor, and 2.75 Gb of RAM. Each deterministic model was solved using the "rolling horizon" strategy introduced in a previous work (Kostin et al., 2011). Specifically, we solved two different case studies that differ in the demand variability. These cases are described in detail next.

Table 5 – Parameters used to evaluate the capital cost for different production technologies.

	α^{PL}_{pgt}, \$	β^{PL}_{pgt}, \$ · year/ton
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 6 – Parameters used to evaluate the capital cost for different storage technologies.

	α^{S}_{sgt}, \$	β^{S}_{sgt}, \$ · year/ton
S1	1,220,000	122
S2	18,940,000	1894

5.1. *High variance in ethanol demand*

In this first case, we consider high and low variabilities for ethanol and sugar demand, respectively. Both parameters are assumed to follow normal distributions with a standard deviation of 30% for ethanol and 5% for sugar.

The resulting non-dominant cumulative risk curves obtained by applying our algorithm are shown in Fig. 7a. Note that each of these curves represents a different SC configuration and associated set of planning decisions for the entire time horizon. As observed, the *NPV* values lie in the interval US$249–616 million. In the figure, we have identified different curves of interest for decision-makers. These are the one with maximum *E*[*NPV*], the deterministic solution (i.e., the one calculated with the deterministic formulation solved for the mean demand), the upper bound risk curve and two curves that may be appealing for risk-averse and risk-takers decision-makers. Let us clarify that the upper bound risk curve does not represent any particular SC configuration. This curve is constructed by plotting the best *NPV* that could be attained in each scenario (i.e., the *NPV* of the best SC configuration for that particular scenario realization). Hence, the upper bound curve represents the best performance that a SC could exhibit in the face of uncertainty (Barbaro and Bagajewicz, 2004).

As observed, the solutions behave in different ways in the face of uncertainty. For instance, for the risk-taker solution, the probability of not exceeding a target value of US$500 million is equal to 77.23%, whereas this probability is gradually decreased to 34.65%, 13.86% and 5.94%, in the deterministic, risk-averse and maximum *E*[*NPV*] solutions, respectively. The maximum *E*[*NPV*] solution is a rather conservative solution that behaves better than the remaining solutions for a wide range of target values on the *NPV*. In fact, there are only 3 solutions out of 72 with lower probabilities of small target values than the maximum expected *NPV* one. Note that the better performance shown by the risk-averse and risk-taker solutions in the lower and upper parts of the prob-

Table 4 – Minimum and maximum production capacities of each technology (ton 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

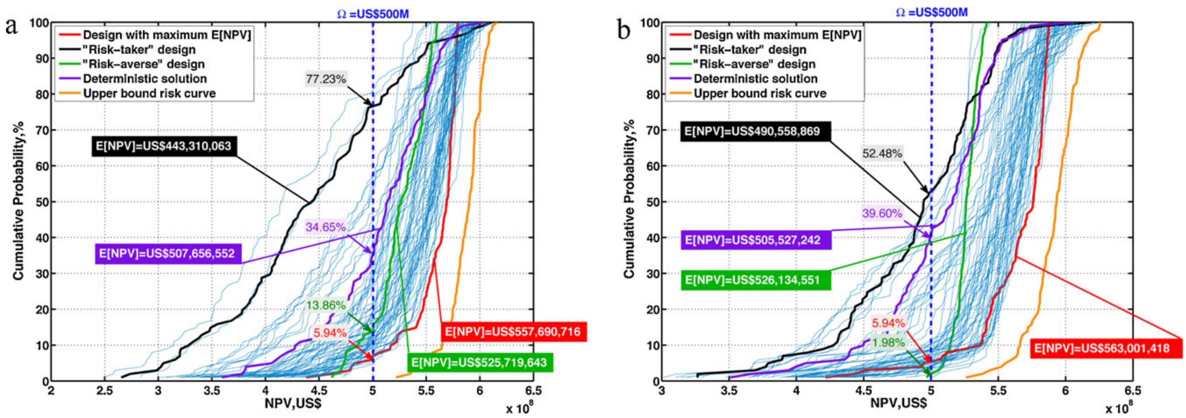

Fig. 7 – (a) Cumulative probability curves for the case of high variance in ethanol demand. (b) Cumulative probability curves for the case of high variance in sugar demand.

ability curves, respectively, is achieved at the expense of a big drop in the expected *NPV*. Particularly, the risk-taker and risk-averse SCs show expected *NPVs* of US$443,310,063, and US$525,719,643, whereas the maximum expected *NPV* is US$557,690,716. In between the risk-taker and risk-averse solution, we can find many SC alternatives behaving in different ways in the face of uncertainty. From these solutions, decision-makers must choose the best one according to their preferences.

Tables 8 and 9 present the structure of the SC associated with the deterministic solution. The design decisions include the construction of 4 sugar mills utilizing technology T2, and 4 distilleries operating with technologies T4 and T5. The production facilities are situated exclusively at the sub-regions of Tucumán and the North West region. 254 medium trucks for sugars and 157 tank trucks for ethanol are purchased to transport the final products from Tucumán and the North West region to the remaining sub-regions. The storages for solid materials (i.e., the ones utilizing technology S1) are present in all sub-regions. Storage facilities for ethanol (i.e., warehouses with technology S2), exist only in 4 sub-regions with comparatively large ethanol demand.

Tables 10, 11 and 12 summarize the SC configurations of the risk-taker, risk-averse and maximum *E[NPV]* solutions, respectively. As shown, the risk-taker configuration shows larger production and transport capacities than the risk-averse and maximum *E[NPV]* designs. On the other hand, it leads to fewer storage facilities. The overall capital expenditures of the risk-averse network are lower than those associated with the remaining solutions, mainly because the extra investment in production plants and transport units is compensated by the savings in storage facilities.

Table 7 – 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)	65	25	28
Availability of transportation mode (h/d)	18	18	18
Cost of establishing transportation mode (US$)	90,000	65,000	100,000
Driver wage (US$/h)	10	10	10
Fuel economy (km/L)	5	5	5
Fuel price (US$/L)	0.85	0.85	0.85
General expenses (US$/d)	8.22	8.22	8.22
Load/unload time of product (h/trip)	6	6	6
Maintenance expenses (US$/km)	0.0976	0.0976	0.0976

Table 8 – Production capacity in the deterministic solution.

Technology	Main product	Number of plants	Sub-region	Capacity, ton of main product/year	Total capacity of main product, ton/year
Deterministic solution: US$1,423,561,900 of capital investments					
T2	White sugar	1	North West	171,958	
T2	White sugar	3	Tucumán	828,042	1,000,000
T4	Ethanol	1	North West	38,498	
T4	Ethanol	1	Tucumán	185,383	
T5	Ethanol	1	North West	272,922	
T5	Ethanol	1	Tucumán	230,116	726,918

Table 9 – Storage capacity in the deterministic solution, ton.

Type	Córdoba	Mesopotamia	Buenos Aires	Cuyo	North	North West	Tucumán	Santa Fe	La Pampa	Santiago	West	Patagonia	Total
S1	4610	4610	24,980	3951	2190	2623	2036	4445	461	1191	1004	2694	54,795
S2	5071	5071	26,804	0	0	2885	0	0	0	0	0	0	39,831

Note that the aforementioned capacities are first-stage variables that limit the potential production rates and storage inventories. According to the demand that finally materializes, the SC can rearrange the materials flows in order to take full advantage of the production and storage capacities. Hence, larger production, transport and storage facilities make it easier to follow a given demand pattern.

Table 13 presents the risk metrics calculated for the different designs. As compared with the risk-taker design, the risk-averse solution offers the maximum reduction in *VaR* from a value of US$137M to US$53M (i.e., a 61.3% reduction). As regards the *OV*, the greatest decrease in this measure can be observed in the solution with the maximum *E*[*NPV*]. Particularly, it reduces the *OV* from a value of US$122M to US$21M (i.e., a 83% reduction). In order to calculate the *RAR*, the risk-taker solution has been chosen as the reference design. As shown, all solution have values of *RAR* much less than 1, and the corresponding cumulative risk curves are positioned almost below the risk-taker one. The risk-averse solution has the greatest value of *RAR* (equal to 0.3). This means that for the risk-averse, maximum *E*[*NPV*] and deterministic solutions the gain in risk reduction is higher than the loss in opportunity.

Figs. 8a, 9a, 10a show the cumulative probability curves of the demand satisfaction levels of white sugar, raw sugar and ethanol, respectively. That is, for a given target on the demand satisfaction level (*x* axis), these figures provide the probability (*y* axis) of achieving a demand satisfaction level less than or equal to that particular target. These curves have been determined for each SC configuration from the sales and demand of sugar and ethanol in each scenario realization. The numbers on these plots show the expected values of the corresponding cumulative probability distributions.

As observed, the curves for white and raw sugar demand satisfaction are rather similar in all the cases (i.e., the expected values do not differ in more than 1.5%). This is because the variability associated with the sugar demand is very low, and all the SC configurations are capable of fulfilling it to a large extent in all the scenarios. In contrast, the ethanol demand satisfaction curves are rather different (expected values in the range 42.1% to 74.5%). The risk-taker SC attains the lowest expected value of ethanol demand satisfaction. This is due to the establishment of only two ethanol storages that allow to cover the demand of only two regions of the country. On the other hand, the design with maximum *E*[*NPV*] leads to the largest ethanol demand satisfaction level. These curves shed light on the performance of each SC configuration under uncertainty. Particularly, the maximum expected *NPV* solution shows better performance in a wide range of *NPV* values due to the establishment of more storage facilities that allow to fulfill the ethanol demand to a larger extent. In contrast, the risk-taker solution invests on fewer storage facilities in order to reduce the capital cost. This leads to larger benefits in scenarios with low demand, but also to poor *NPV*s when large demands are materialized.

Comparing the solutions generated by the SAA with the deterministic one, it is observed that there are 60 out of 72 SC configurations that yield better performance than the deterministic design. Furthermore, the expected *NPV* in the deterministic case is US$50,034,164 lower than that attained by the maximum expected *NPV* solution identified by the SAA. With regard to the shape of the risk curves, the deterministic solution leads to a risk-averse probability curve.

Table 10 – Production capacities for risk-taker, risk-averse and maximum *E*[*NPV*] solutions for the case of high variance in ethanol demand.

Technology	Main product	Number of plants	Sub-region	Capacity, ton of main product/year	Total capacity of main product, ton/year
Risk-taker solution: US$1,388,582,700 of capital investments					
T2	White sugar	1	North West	174,777	
T2	White sugar	3	Tucumán	813,576	988,354
T4	Ethanol	1	North West	39,129	
T4	Ethanol	1	Tucumán	182,144	
T5	Ethanol	1	North West	271,275	
T5	Ethanol	1	Tucumán	236,565	731,113
Risk-averse solution: US$1,498,569,200 of capital investments					
T2	White sugar	1	North West	286,477	
T2	White sugar	2	Tucumán	700,000	986,477
T4	Ethanol	1	North West	64,137	
T4	Ethanol	1	Tucumán	156,716	
T5	Ethanol	1	North West	206,030	
T5	Ethanol	1	Tucumán	300,000	726,883
Maximum *E*[*NPV*] solution: US$1,457,363,600 of capital investments					
T2	White sugar	1	North West	282,176	
T2	White sugar	2	Tucumán	700,000	982,176
T4	Ethanol	1	North West	63,174	
T4	Ethanol	1	Tucumán	156,716	
T5	Ethanol	1	North West	208,621	
T5	Ethanol	1	Tucumán	300,000	728,511

Table 11 – Storage capacities for risk-taker, risk-averse and maximum *E*[*NPV*] solutions for the case of high variance in ethanol demand, ton.

Type	Córdoba	Mesopotamia	Buenos Aires	Cuyo	North	North West	Tucumán	Santa Fe	La Pampa	Santiago	West	Patagonia	Total
Risk-taker solution													
S1	4838	5080	24,304	4388	2386	2876	2094	4566	465	1225	1027	2710	55,959
S2	0	4910	36,093	0	0	0	0	0	0	0	0	0	41,003
Risk-averse solution													
S1	4686	4983	25,107	4058	2154	2816	2231	4551	495	1272	1072	2797	56,224
S2	6909	4754	12,605	5350	0	3970	2838	6032	0	0	0	4085	46,543
Maximum *E*[*NPV*] solution													
S1	4537	4688	25,867	3867	2214	2707	2116	4717	487	1254	993	2848	56,295
S2	5776	5129	22,048	3582	0	3821	0	4250	0	0	0	0	44,605

5.2. *High variance in sugar demand*

In this case, we assume a standard deviation equal to 30% for white and raw sugars demands and 5% for ethanol demand. The resulting non-dominant cumulative risk curves are presented in Fig. 7b. As compared to the case of high variance in ethanol demand, the resulting values of *NPV* under high variance in sugar demand show a narrower interval that goes from US$301 to US$626 million. The risk of not exceeding the target of $500 million in the risk-taker solution is equal to 52.48%. In the deterministic, the maximum *E*[*NPV*], and the risk-averse solutions these probabilities are equal to 39.60%, 5.94%, 1.98%, respectively. As happened previously, the solution with the maximum *E*[*NPV*] behaves quite conservatively, and there are only 12 out of 68 non-dominant solutions with lower probabilities of small target values than the maximum expected *NPV* one.

Table 12 – Number of transportation vehicles for risk-taker, risk-averse and maximum *E*[*NPV*] solutions for the case of high variance in ethanol demand.

Design	Heavy truck	Medium truck	Tank truck
Risk-taker	0	248	187
Risk-averse	0	255	142
Maximal *E*[*NPV*]	0	257	151

Tables 14, 15 and 16 present the resulting first-stage variables of the SC configurations obtained for the risk-taker, risk-averse and maximum *E*[*NPV*] solutions. As observed, all the networks involve highly centralized organizations with a tendency to build the sugar mills and the distilleries in the sub-regions with their own sugar cane plantations. Particulary, the model decides to install production facilities only in the sub-regions with large sugar cane capacities namely Tucumán and North West.

Regarding storage, all the configurations have storages for sugars. Thereby, the main factor causing different shapes and slopes of the risk curves in the case of high variance in sugar demand is the sugar production capacity. As shown, the risk-

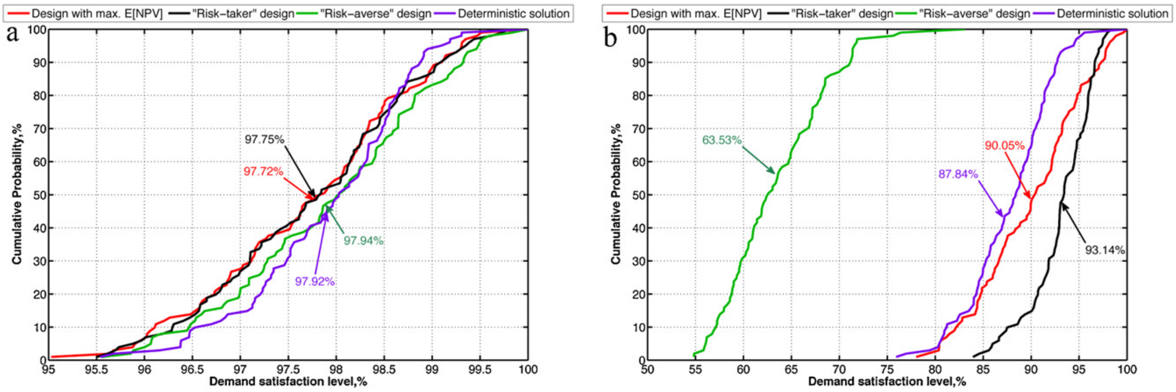

Fig. 8 – (a) Cumulative probability curves for white sugar demand satisfaction level under high variance in ethanol demand. (b) Cumulative probability curves for white sugar demand satisfaction level under high variance in sugar demand.

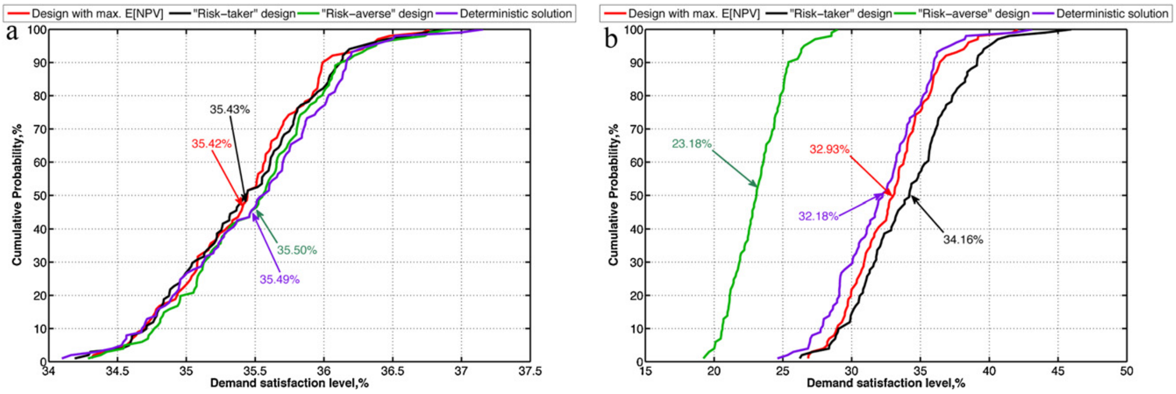

Fig. 9 – (a) Cumulative probability curves for raw sugar demand satisfaction level under high variance in ethanol demand. (b) Cumulative probability curves for raw sugar demand satisfaction level under high variance in sugar demand.

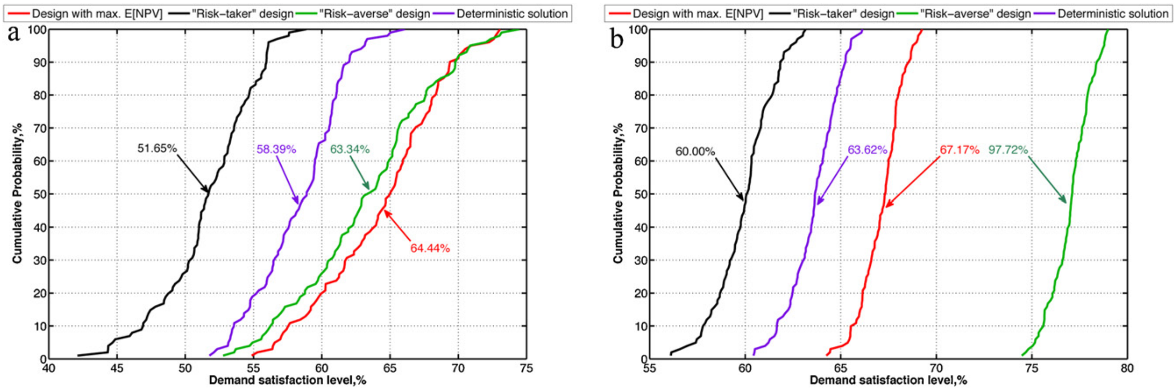

Fig. 10 – (a) Cumulative probability curves for ethanol demand satisfaction level under high variance in ethanol demand. (b) Cumulative probability curves for ethanol demand satisfaction level under high variance in sugar demand.

Table 13 – Values of *VaR*, *OV* and *RAR* to risk-taker design for the selected solutions, US$.

	Type of solution			
	Risk-taker	Risk-averse	Maximum *E*[*NPV*]	Deterministic
High variance in ethanol demand				
VaR	138,615,053	52,530,213	75,025,076	101,789,033
OV	121,911,937	32,622,837	20,945,374	62,400,497
RAR	–	0.30	0.09	0.17
High variance in sugar demand				
VaR	111,538,469	16,744,581	68,545,708	98,746,232
OV	65,834,581	12,203,389	23,312,212	47,085,358
RAR	–	0.17	0.01	0.10

Table 14 – Production capacities for risk-taker, risk-averse and maximum *E*[*NPV*] solutions for the case of high variance in white and raw sugars demand.

Technology	Main product	Number of plants	Sub-region	Capacity, ton of main product/year	Total capacity of main product, ton/year
Risk-taker solution: US$1,440,257,000 of capital investments					
T2	White sugar	1	North West	204,605	
T2	White sugar	3	Tucumán	886,013	1,090,618
T4	Ethanol	1	North West	45,807	
T4	Ethanol	1	Tucumán	198,361	
T5	Ethanol	1	North West	253,852	
T5	Ethanol	1	Tucumán	196,254	694,275
Risk-averse solution: US$1,406,887,800 of capital investments					
T2	White sugar	1	North West	301,103	
T2	White sugar	1	Tucumán	350,000	651,103
T4	Ethanol	1	North West	67,411	
T4	Ethanol	1	Tucumán	78,358	
T5	Ethanol	1	North West	197,487	
T5	Ethanol	2	Tucumán	509,346	852,602
Maximum *E*[*NPV*] solution: US$1,415,866,400 of capital investments					
T2	White sugar	1	North West	232,327	
T2	White sugar	2	Tucumán	700,000	932,327
T4	Ethanol	1	North West	52,013	
T4	Ethanol	1	Tucumán	156,716	
T5	Ethanol	1	North West	237,660	
T5	Ethanol	1	Tucumán	300,000	746,390

Table 15 – Storage capacities for risk-taker, risk-averse and maximum *E*[*NPV*] solutions at the case of high variance in white and raw sugars demand, ton.

Type	Córdoba	Mesopotamia	Buenos Aires	Cuyo	North	North West	Tucumán	Santa Fe	La Pampa	Santiago	West	Patagonia	Total
Risk-taker solution													
S1	7000	5803	28,314	6961	3179	3641	3067	6418	606	1107	1443	2088	69,628
S2	5159	5082	25,368	0	0	3069	0	0	0	0	0	0	38,678
Risk-averse solution													
S1	6347	4426	10,677	6315	2379	3059	2509	6320	452	1538	1350	3167	48,539
S2	5127	5002	24,898	4208	0	3048	0	4972	0	0	0	0	47,254
Maximum *E*[*NPV*] solution													
S1	5779	5401	58,772	4947	2528	9650	2636	4979	568	1444	1227	34,947	132,879
S2	5151	5065	26,786	0	0	0	0	5040	0	0	0	0	42,042

Table 16 – Number of transportation vehicles for risk-taker, risk-averse and maximum *E*[*NPV*] solutions for the case of high variance in sugar demand.

Design	Heavy truck	Medium truck	Tank truck
Risk-taker	0	281	149
Risk-averse	0	162	175
Maximal *E*[*NPV*]	0	239	171

taker solution has the largest production capacity of white and raw sugar and the lowest ethanol production capacity. In contrast, the configuration from the risk-averse solution is ethanol-oriented. The probability curves for white sugar, raw sugar and ethanol demand satisfaction levels are shown in Figs. 8b, 9b and 10b, respectively. As observed, the risk-taker design attains the highest expected demand satisfaction of white and raw sugar, whereas the risk-averse configuration shows the largest ethanol demand satisfaction level.

Comparing the solutions generated by the SAA algorithm with the deterministic one, we see that there are 60 out of 68 SC configurations that yield better performance than the deterministic design. Furthermore, the expected *NPV* in the deterministic case is US$57,474,176 lower than that attained by the maximum expected *NPV* solution identified by the SAA. Regarding the shape of the risk curves, the deterministic solution results in a risk-taker probability curve.

As regards the risk metrics, the risk-averse solution leads to the largest decrease in both *VaR* and *OV* values (see Table 13). Particularly, It reduces the value at risk from US$112M to US$17M (85% reduction). The value of *OV* is decreased from US$67M to US$12M (82% reduction). In addition, the risk area for this solution is the largest one (i.e., 0.17).

6. Conclusions

In this work, we have proposed a two-stage stochastic mixed-integer linear programming approach for the optimal design and planning of bioethanol SCs under uncertainty in product demand. The problem was solved applying the SAA algorithm, which provides as output a set of SC configurations that behave in different ways in the face of uncertainty.

A real case study based on the current Argentinean sugar cane industry has been presented to show the capabilities of our approach. Since the final products of the sugar cane industry in Argentina are sugar and bioethanol, we developed two different case studies that differ in the variance of the uncertain sugar and ethanol demands. Numerical results show that the centralized production is more favorable. Furthermore, the production facilities should be located close to the sugar cane plantations. Among the technologies that convert sugar cane to white and raw sugars the one producing honey as a by-product is preferable. In addition, it is concluded that ethanol should be produced by fermentation of sugarcane juice or honey from sugar mills.

We have shown that the SAA is able to provide solutions that behave better than the deterministic one in the face of uncertainty (i.e., solutions yielding better expected *NPV* than that associated with the deterministic one). The proposed methodology offers different risk-related alternatives for decision-making. The analysis of the stochastic results reveals that there are two critical factors that influence the SC performance under uncertainty. The first one is the production capacity. As a rule, risk-taker SC configurations imply production facilities with larger capacities. The second one is the amount of storages and transportation units. SCs with larger number of warehouses and trucks provide more flexibility to rearrange products flows, which makes it easier to implement risk-averse manufacturing policies. These configurations, however, require larger capital investments and therefore lead to lower profits. The tool presented in this work is intended to help policy makers in the strategic planning of infrastructures for ethanol and sugar production in the face of uncertainity.

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Appendix A. Supplementary Data

Supplementary data associated with this article can be found, in the online version, at doi:10.1016/j.cherd.2011.07.013.

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9.3 Multi-objective model for more sustainable fuel supply chains. A case study of the sugarcane industry in Argentina

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

Fernando D. Mele,*,† Andrew M. Kostin,‡ Gonzalo Guillén-Gosálbez,‡ and Laureano Jiménez‡

†Departamento de Ingeniería de Procesos, FACET, Universidad Nacional de Tucumán (UNT), Avenida Independencia 1800, S. M. de Tucumán T4002BLR, Argentina

‡Departament d'Enginyeria Química (EQ), Escola Tècnica Superior d'Enginyeria Química (ETSEQ), Universitat Rovira i Virgili (URV), Campus Sescelades, Avinguda Països Catalans, 26, 43007 Tarragona, Spain

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.[1] Von Blottnitz and Curran[2] 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-Álcohol 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.[3] 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.[4]

Many countries have launched programs to replace gasoline by ethanol in the midterm. China, India, Colombia, Thailand, Mexico, and Venezuela[5] 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.[6] 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, SOx 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.[7]

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.[8] An extensive review with more than 200 citations related to GrSCM can be found in the work by Srivastava.[9] 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.[10] 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.[11] presented an LP model to minimize the transportation and storage costs of the existing sugar cane SC in Brazil. Ioannou[12] 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.[13] minimizes the transportation cost of the sugar cane SC in Cuba. Dunnett[14] et al. developed a model to find the optimal configuration of a lignocellulosic bioethanol network. Zamboni et al.[15] 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.,[16] Paiva and Morabito,[17] Colin,[18] and Higgins and Laredo.[19] 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,[20] a framework that was formally introduced by Azapagic and Clift.[21] This integrated framework allows an automation of the search for alternatives leading to life cycle environmental savings. The works by Hugo and Pistikopoulos,[22] Bojarski et al.,[23] and Guillén-Gosálbez et al.[24] are examples of the application of this general approach to process industries. Very few works have addressed the multiobjective optimization of bioethanol SCs with economic and LCA-based criteria. Buddadee et al.[25] 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.[26] presented a multiobjective framework to optimize the design of the corn-based ethanol SC in northern Italy, as an extension of a former article.[15] They also considered economic and environmental metrics in the optimization.

In contrast to these approaches, the works by Beeharry,[27] Ramjeawon,[28] Botha and von Blottnitz,[29] and Renouf et al.[30] focused on assessing the life cycle impact of ethanol production from sugar cane. In the same line, Contreras et al.[31] 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.

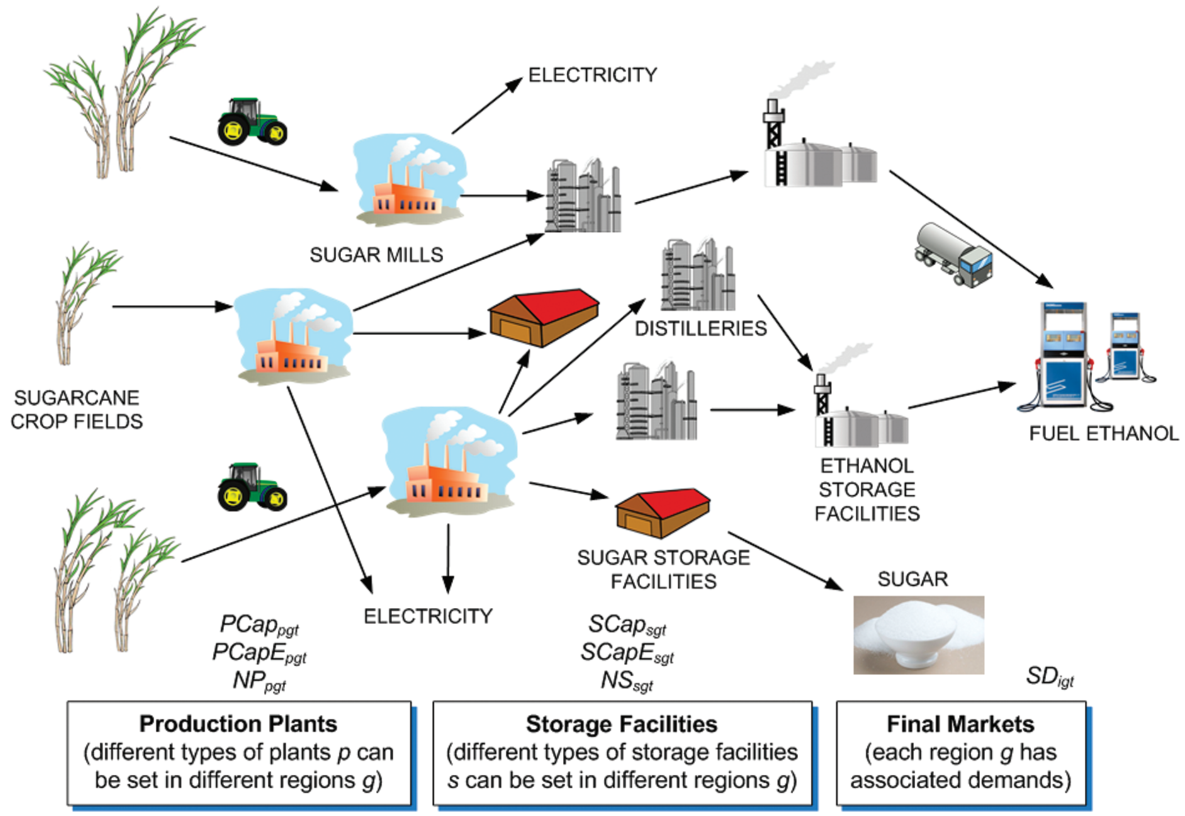

Figure 1. Structure of the bioethanol/sugar SC.

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.[24,32] Here, we integrate our LCA analysis with multiobjective optimization, following the approach introduced by Azapagic and Clift.[21] Examples on the application of this general framework to other cases can be found elsewhere.[8,22,24,33−36]

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).[37] 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.[38]

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.

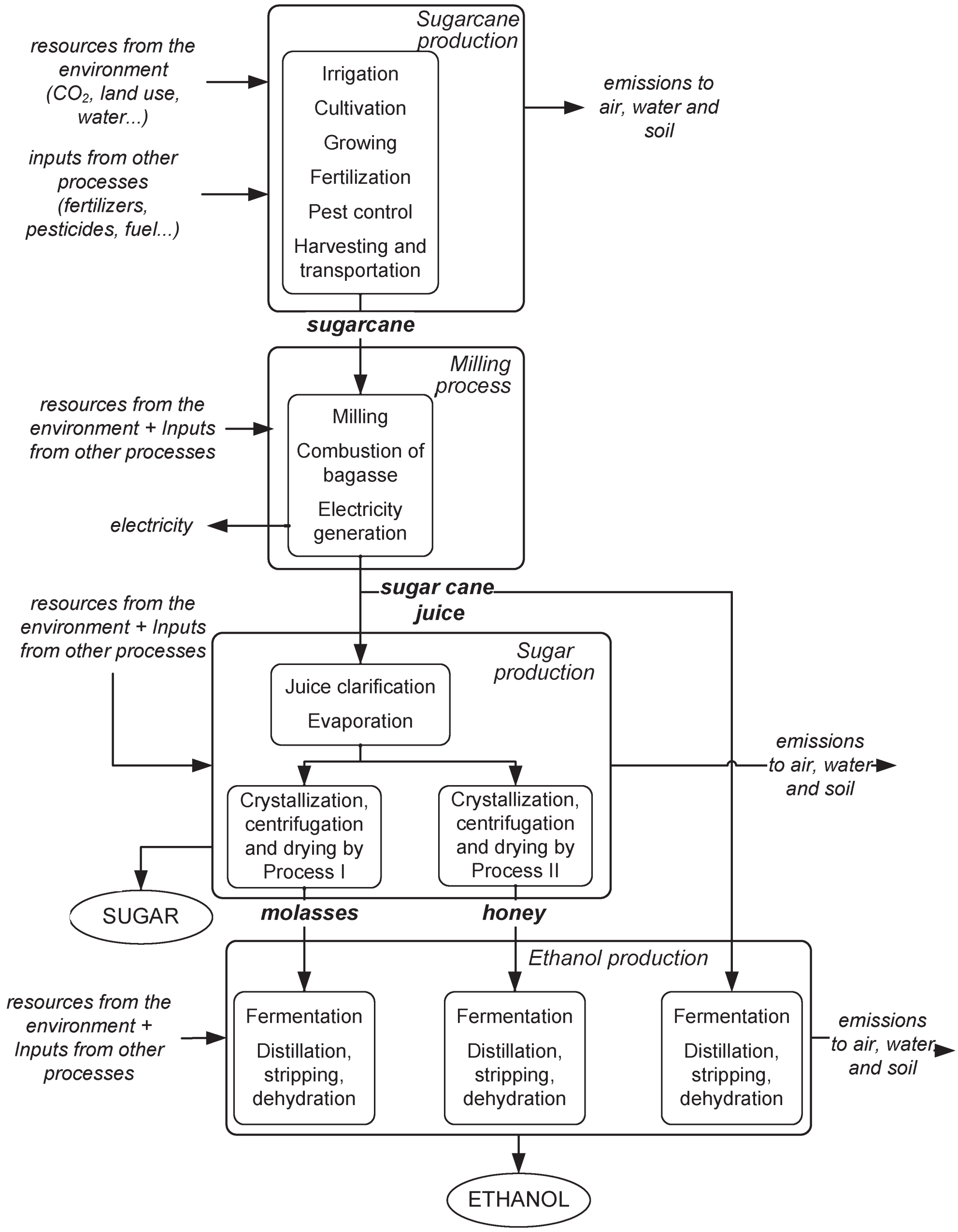

Figure 2. System boundaries considered in the LCA study.

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[45]
CO_2	0.8195	t[a]
O_2	0.1631	t[a]
fueloil	1.7807	t[39]
from the technosphere		
urea	2.9851	kg[b]
superphosphate	0.3582	kg[b]
pesticides	0.2687	kg[b]
filter muds	0.04	t[b]
Outputs		
emissions to the water		
pesticides	0.0009	kg[30]
PO_4^{3-}	0.3821	kg[30]
NO_3^-	0.194	kg[30]
emissions to the air		
O_2	0.596	t[a]
CO_2	192.5513	kg[a]
CO	21.7362	kg[a]
NO_x	1.024	kg[30]
SO_x	0.062	kg[39]
N2O	0.2	kg[30]
NH_3	0.0776	kg[30]
particles	15.004	kg[b]
emissions to the soil		
ash	5.673	kg[b]
harvest trash	155	kg[b]
products		
sugar cane	1	t

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

Table 2. Summary of the Inventory Data for Subsystem Milling

	quantity	unit
Inputs		
from the ecosphere		
water	0.4078	t[a]
O_2	0.0998	t[a]
from the technosphere		
harvested sugar cane	1	t
Outputs		
emissions to the water		
solids	0.0019	t[46]
emissions to the air		
CO_2	0.2580	t[a]
NO_x	0.0002	t[46]
SO_x	0.0001	t[46]
particles	0.0002	t[46]
emissions to the soil		
boiler ash	0.0366	t[b]
products		
electricity to the process	54	MJ[b]
electricity for export	132.12	MJ[b]
LP steam to the process	0.5040	t[b]
sugar cane juice	0.8976	t[b]
bagasse excess	0.02	t[b]

[a] Carbon balance calculations (combustion). [b] 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[a]	steam	3.7290	t[a]
lime	16.6667	kg[a]	lime	20	kg[a]
sulfur	2.5	kg[a]	sulfur	3	kg[a]
O_2	4.5	kg[a]	O_2	5.4	kg[a]
flocculant	0.001	kg[30]	flocculant	0.0012	kg[30]
NaOH	0.0014	t[a]	NaOH	0.0016	t[a]
HCl	0.0027	t[a]	HCl	0.0032	t[a]
Outputs					
emissions to the water			emissions to the water		
BOD_5	0.0021	kg[30]	BOD_5	0.0026	kg[30]
suspended solids	0.0032	kg[30]	suspended solids	0.0039	kg[30]
inorganic solubles	0.0696	t[39]	inorganic solubles	0.0835	t[39]
emissions to the air			emissions to the air		
SO_x	0.5	kg[39]	SO_x	0.6	kg[39]
products			products		
white sugar	1	t	white sugar	1	t
raw sugar	0.176	t[a]	raw sugar	0.18	t[a]
molasses	0.4167	t[a]	honey	0.75	t[a]
filter muds	0.3333	t[47]	filter muds	0.4	t[47]

[a] 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.[39]

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_2, 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.

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[a]

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_3PO_4	0.0004	t	H_3PO_4	0.0004	t	H_3PO_4	0.0004	t
water	1.84	t	water	1.84	t	water	1.84	t
H_2SO_4	0.013	t	H_2SO_4	0.013	t	H_2SO_4	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[48]
pH	4.9		pH	4.8		pH	4.6	
DQO	1.4516	t	DQO	1.4515	t	DQO	1.4516	t
DBO_5	0.5267	t	DBO_5	0.5267	t	DBO_5	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_2	3.37	t	CO_2	3.37	t	CO_2	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

[a] 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.[39] 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.[40] 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.[21,22,24,26] 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,[41] and Guillén-Gosálbez et al.,[24] 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.[8]

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.

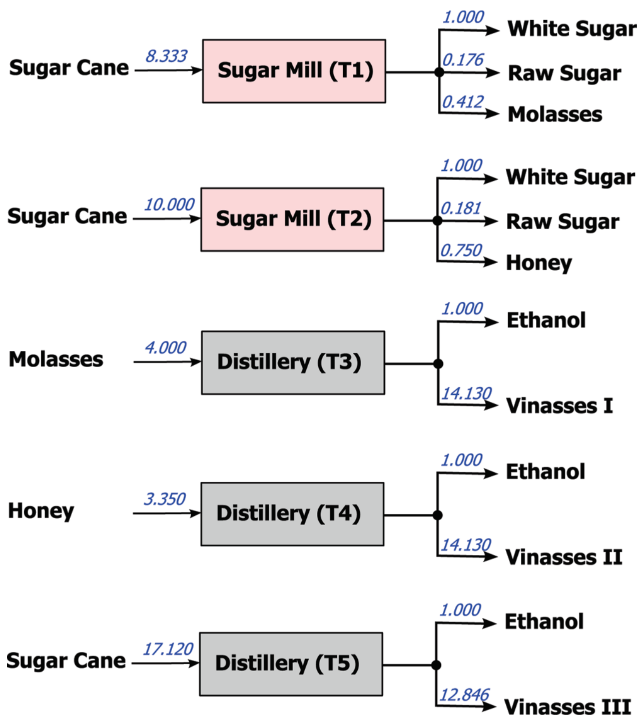

Figure 3. Schematic representation of the five production technologies considered in the SC model with corresponding mass coefficients.

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 ($Q_{ilg'gt}$), 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}).

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

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:

$$PT_{igt} = \sum_{p} PE_{ipgt} \quad \forall\ i, g, t \tag{2}$$

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, ρ_{pi}, and the production rate of the main products:

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

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:

$$PU_{igt} \le CapCrop_{gt} \qquad i = \text{sugarcane}, \quad \forall\, g, t \tag{4}$$

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

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

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 σ:

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

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.[42]

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

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

$$DTS_{igt} \le SD_{igt} \quad \forall\, i, g, t \tag{8}$$

The existence of a transportation link between two regions g and g' is represented by a binary variable $X_{lgg't}$ 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:

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

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, τ, multiplied by the existing capacity (represented by the continuous variable $PCap_{pgt}$) and the maximum capacity:

$$\tau PCap_{pgt} \le PE_{ipgt} \le PCap_{pgt} \quad \forall\, i, p, g, t \tag{10}$$

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 ($PCapE_{pgt}$):

$$PCap_{pgt} = PCap_{pgt-1} + PCapE_{pgt} \quad \forall\, p, g, t \tag{11}$$

Equation 12 limits the capacity expansions $PCapE_{pgt}$ between upper and lower bounds, denoted by $\underline{PCap}_p$ and $\overline{PCap}_p$, respectively. This equation makes use of the integer variable NP_{pgt}, which denotes the number of plants installed in region g and time period t.

$$\underline{PCap}_p NP_{pgt} \le PCapE_{pgt} \le \overline{PCap}_p NP_{pgt} \quad \forall\, p, g, t \tag{12}$$

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 ($SCapE_{sgt}$):

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

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

$$\underline{SCap}_s NS_{sgt} \le SCapE_{sgt} \le \overline{SCap}_s NS_{sgt} \quad \forall\, s, g, t \tag{14}$$

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

$$\underline{Q}_l X_{lgg't} \le \sum_{i \in IL(i,l)} Q_{ilgg't} \le \overline{Q}_l X_{lgg't} \quad \forall\, l, t, g, g'(g' \ne g) \tag{15}$$

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:

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

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:

$$CF_t = NE_t - FTDC_t \quad t = 1, \ldots, T-1 \tag{17}$$

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.

$$CF_t = NE_t - FTDC_t + svFCI \quad t = T \tag{18}$$

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:

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

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

Table 5. Environmental Impact Factors, υ_b

product	subsystem	unit	GWP100 kg CO_2 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[39]	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

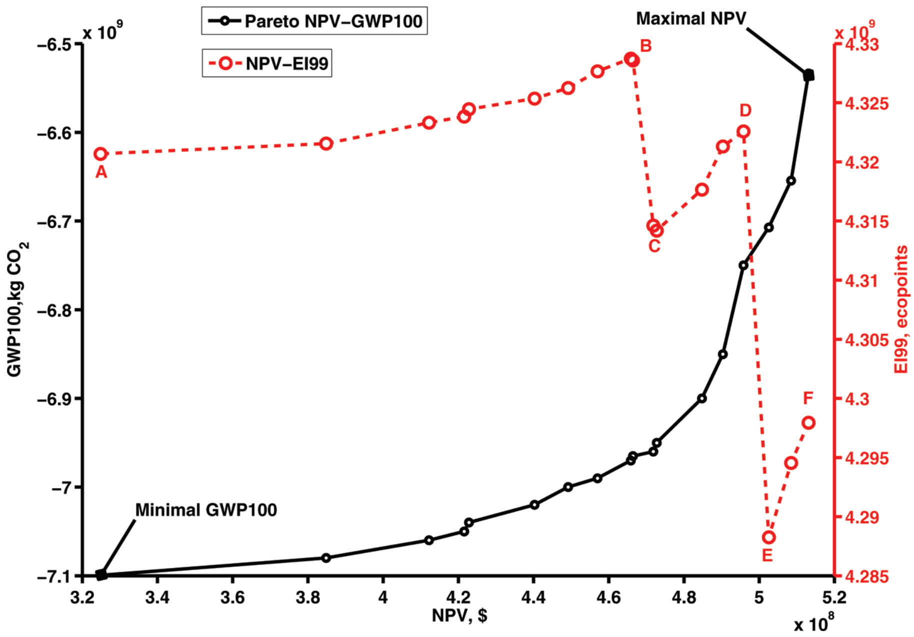

Figure 4. Pareto set of solutions GWP100 vs NPV, and corresponding values of EI99.

prices (PR_{igt}):

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

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):

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

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

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

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

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

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

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

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 ($Q_{ilgg't}/TCap_l$). 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):

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

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:

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

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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:

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

The depreciation term is calculated with the straight-line method, similarly as in other SCM models available in the literature:[8,22]

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

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:

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

Here, the parameters α^{Pr}_{pgt}, β^{Pr}_{pgt} and α^{St}_{sgt}, β^{St}_{sgt} 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:

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

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

$$FCI \leq \overline{FCI} \tag{31}$$

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

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

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.

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

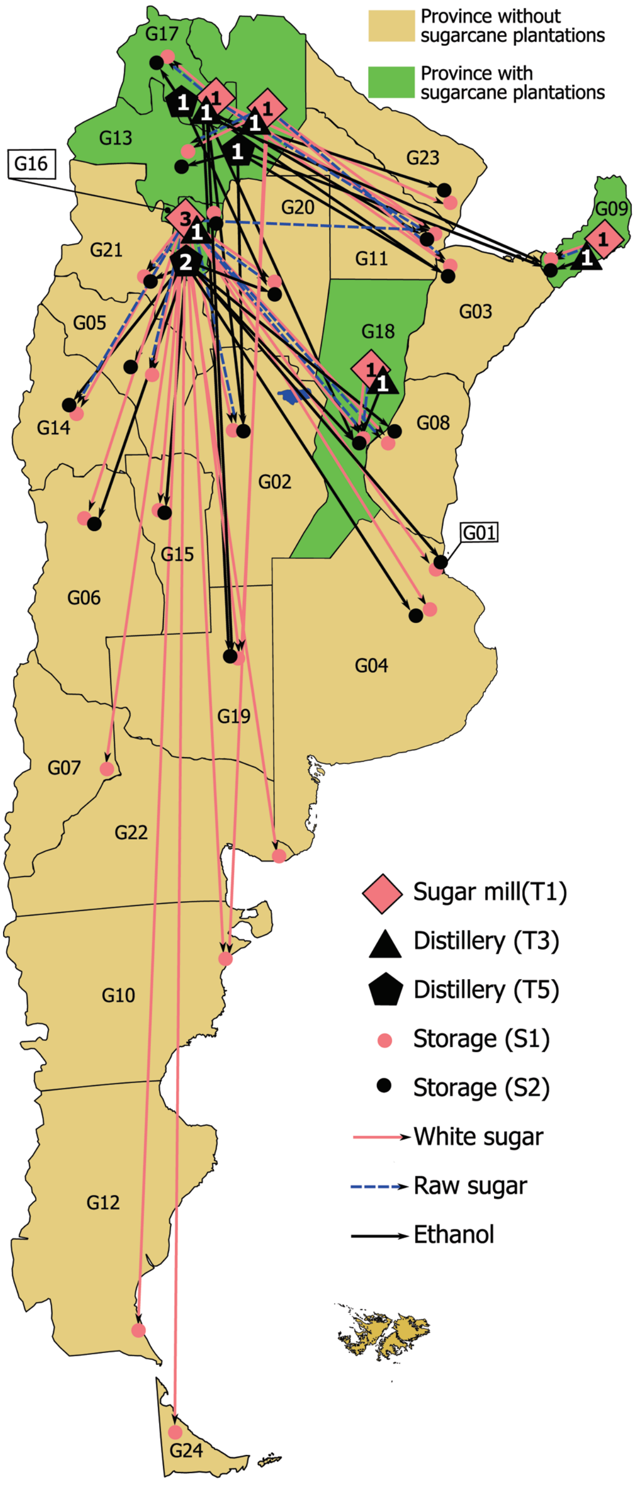

Figure 5. SC configuration of the minimum GWP100 solution.

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. ω^{Pr}_{bp} and ω^{Tr}_b denote the life cycle inventory entries (i.e., emissions released to the environment or resource taken from the ecosphere) associated with

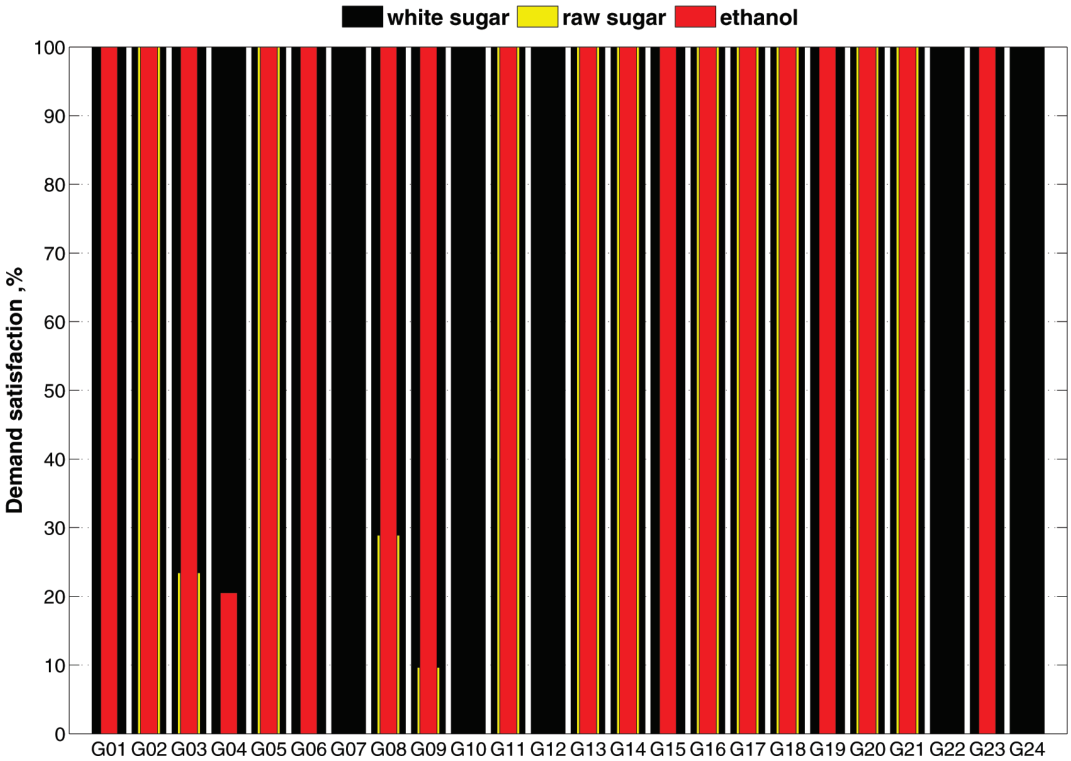

Figure 6. Demand satisfaction level associated with the minimum GWP100 solution.

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 (υ_b), as stated in equation eq 34,

$$\text{DAM} = \sum_b \upsilon_b \cdot \text{LCI}_b \qquad (34)$$

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

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

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

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 ε-constraint method,[43] which entails solving a set of instances of the following single-objective problem M1 for different values of the auxiliary parameter ε:

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

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

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

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

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

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

■ 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[44] and solved with the MILP solver CPLEX 11.0 on a HP Compaq DC5850 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_2 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_2 emissions (8%, from -7.1×10^9 kg CO_2 to -6.5×10^9 kg CO_2).

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_2 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 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

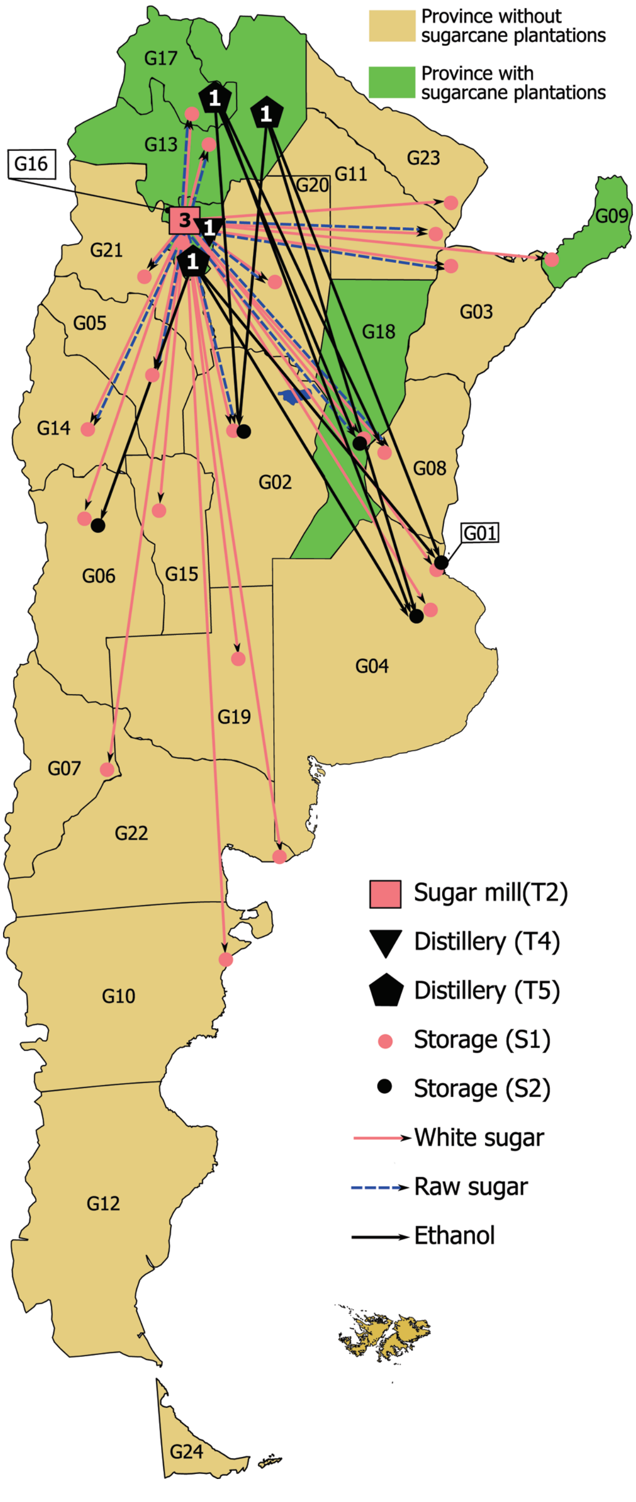

Figure 7. SC configuration of the maximum NPV solution.

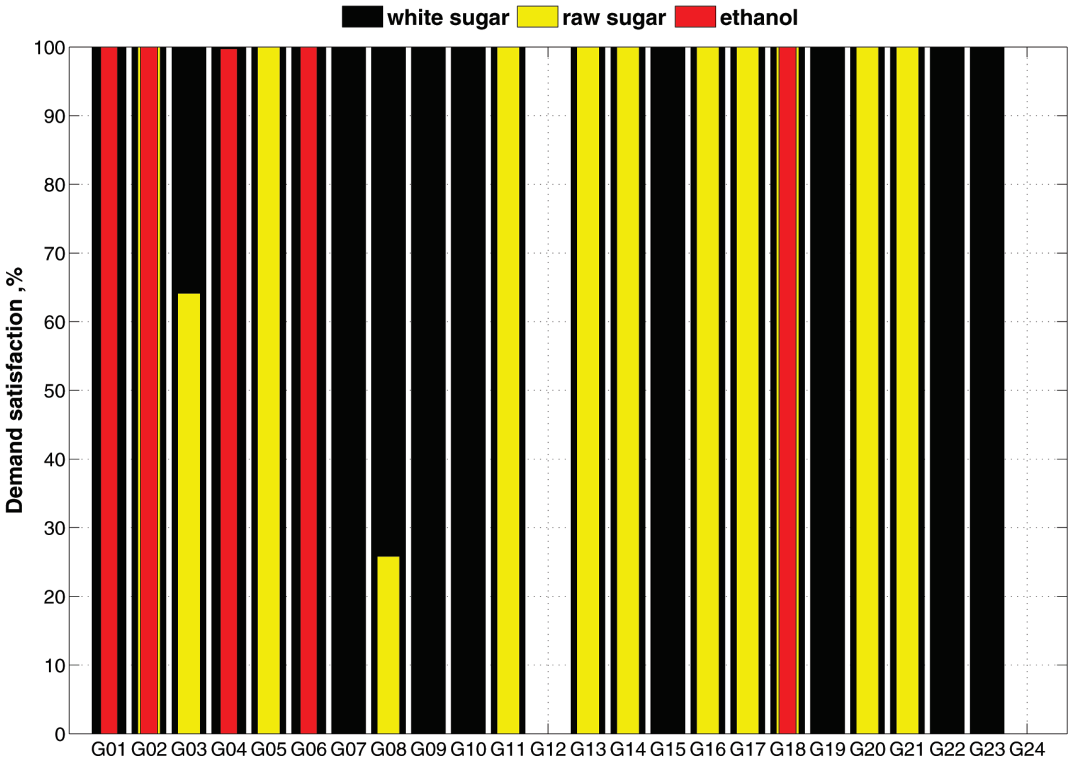

Figure 8. Demand satisfaction level associated with the maximum NPV solution.

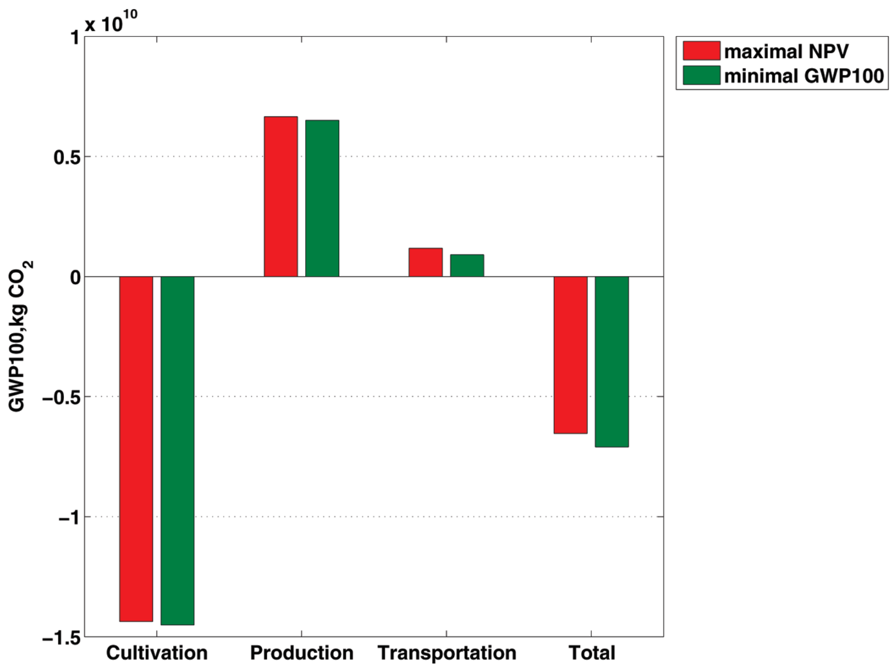

Figure 9. Contribution of different SC stages to the GWP100 for the extreme solutions.

solution, storage facilities are opened as close as possible to the plants in order to minimize the CO_2 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

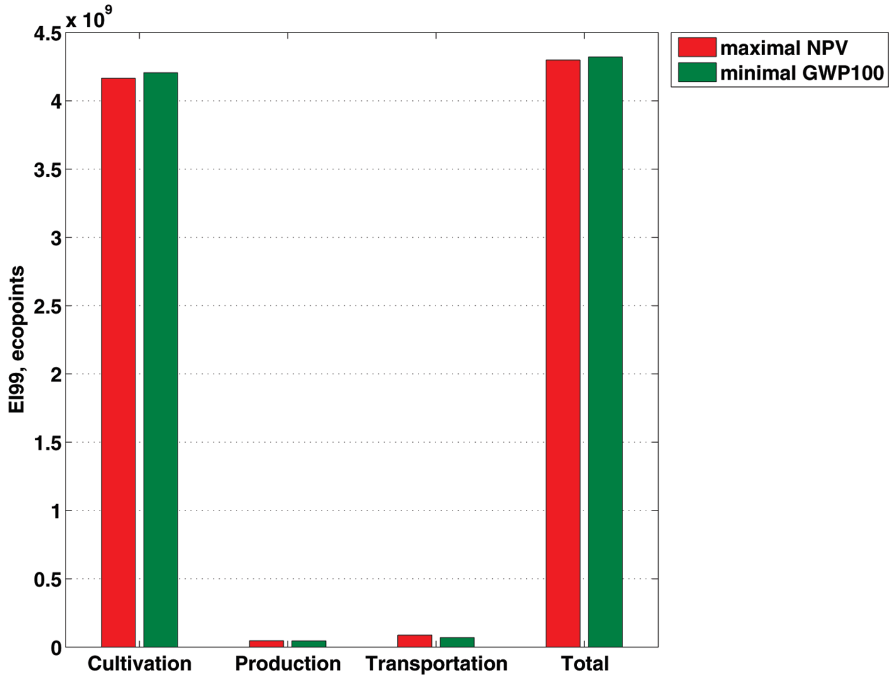

Figure 10. Contribution of different SC stages to the EI99 for the extreme solutions.

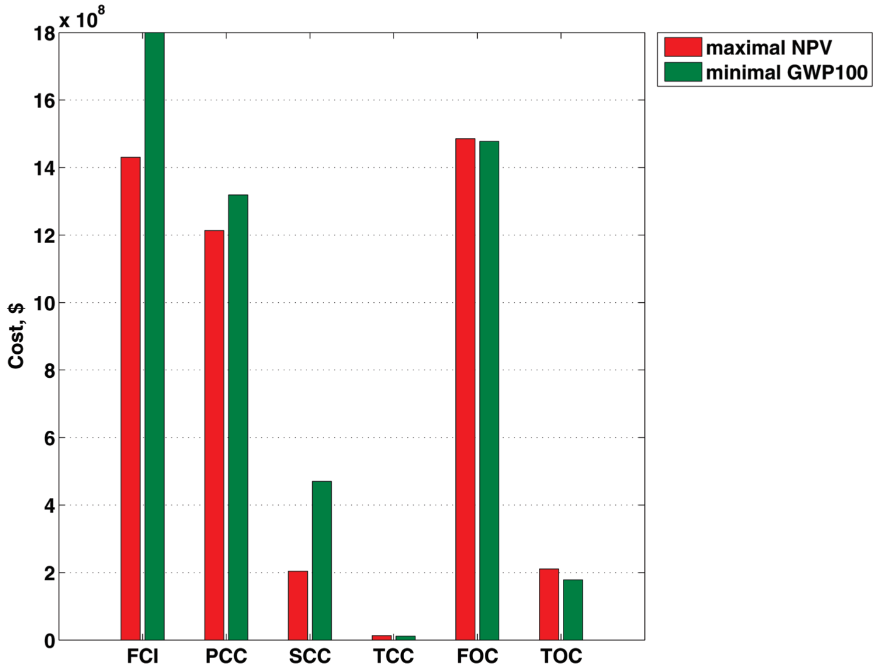

Figure 11. Breakdown of total cost into facility capital investment (FCI), plant capital cost (PCC), storage capital cost (SCC), transportation capital cost (TCC), facility operating cost (FOC) and transportation operating cost (TOC) for the extreme solutions.

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_2 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

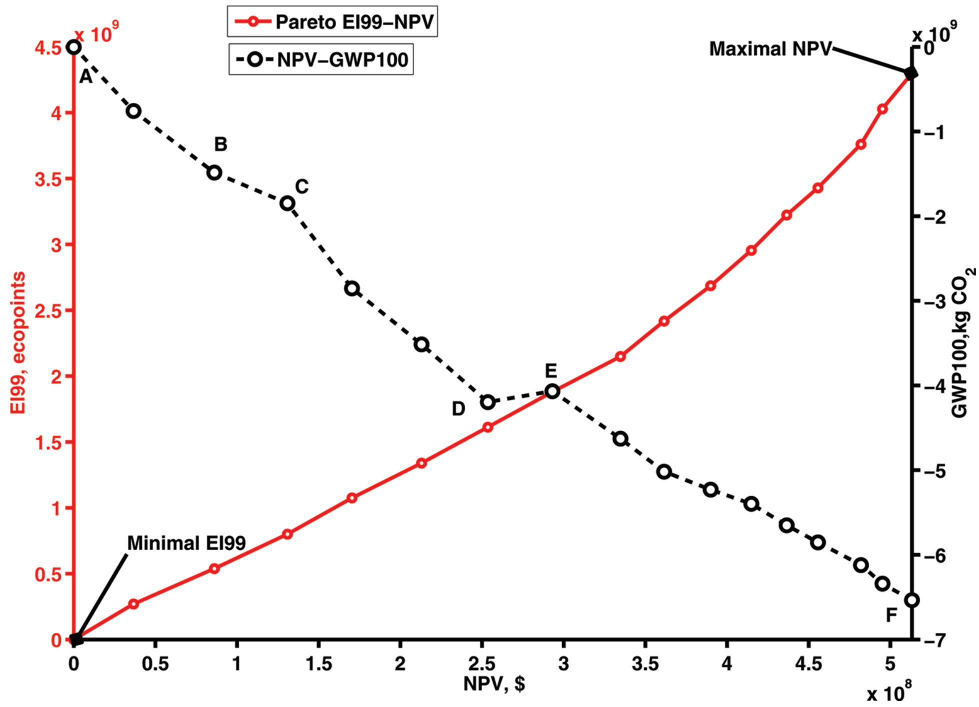

Figure 12. Pareto set of solutions EI99 versus NPV, and corresponding values of GWP100.

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_2 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	680	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	2 356	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

	α_{pgt}^{Pr} (\$)	β_{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

	α_{sgt}^{St} (\$)	β_{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 (τ) has been fixed to zero, and the storage period (σ) 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 (φ), 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).

AUTHOR INFORMATION

Corresponding Author
*E-mail: fmele@herrera.unt.edu.ar.

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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

α^{Pr}_{pgt} = fixed investment coefficient for technology p
α^{St}_{sgt} = fixed investment coefficient for storage technology s
β^{Pr}_{pgt} = variable investment coefficient for technology p
β^{St}_{sgt} = variable investment coefficient for storage technology s
ε = auxiliary boundary for the ε-constraint method
ρ_{pi} = material balance coefficient associated with material i and technology p
σ = storage period
τ = minimum desired percentage of the available installed capacity that must be utilized
υ_b = damage factor associated to chemical specie b
φ = tax rate
ω^{Pr}_{bp} = life cycle environmental burden associated to chemical b (production stage)
ω^{Tr}_{b} = life cycle environmental burden associated to chemical b (transportation stage)
avl_l = availability of transportation mode l
$\mathrm{CapCrop}_{gt}$ = total capacity of sugar cane plantations in region g in time t
DW_{lt} = driver wage
$\mathrm{EL}_{gg'}$ = distance between g and g'
$\overline{\mathrm{FCI}}$ = 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
$\overline{\mathrm{PCap}}_p$ = maximum capacity of technology p
$\underline{\mathrm{PCap}}_p$ = minimum capacity of technology p
PR_{igt} = prices of final products
$\overline{Q}_l$ = maximum capacity of transportation mode l
$\underline{Q}_l$ = minimum capacity of transportation mode l
$\overline{\mathrm{SCap}}_s$ = maximum capacity of storage technology s
$\underline{\mathrm{SCap}}_s$ = 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
$Q_{ilgg't}$ = 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
$X_{lgg't}$ = 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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9.4 Identifying key life cycle assessment metrics in the multi-objective design of bioethanol supply chains using a rigorous mixed integer linear problem approach.

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Identifying Key Life Cycle Assessment Metrics in the Multiobjective Design of Bioethanol Supply Chains Using a Rigorous Mixed-Integer Linear Programming Approach

A. Kostin,[†] G. Guillén-Gosálbez,[†,*] F. D. Mele,[‡] and L. Jiménez[†]

[†]Departament d'Enginyeria Química (EQ), Escola Tècnica Superior d'Enginyeria Química (ETSEQ), Universitat Rovira i Virgili (URV), Campus Sescelades, Avinguda Països Catalans, 26, 43007 Tarragona, Spain

[‡]Dpto. Ingeniería de Procesos, FACET, Universidad Nacional de Tucumán (UNT), Av. Independencia 1800, S. M. de Tucumán T4002BLR, Argentina

ABSTRACT: The design of more sustainable bioethanol supply chains (SCs) has recently emerged as an active area of research. Most of the approaches presented so far have somehow a limited scope, as they focus on minimizing the emitted greenhouse gases as unique criterion, neglecting the damage caused in other impact categories. In this work, we address the multiobjective design of bioethanol SCs considering several life cycle assessment impacts. To overcome the numerical difficulties of dealing with several objective functions, we investigate the application of a rigorous mixed-integer linear programming-based dimensionality reduction method that minimizes the error of omitting objectives. The usefulness of this approach is tested through its application to the design of a bioethanol/sugar SC in Argentina, in which five environmental objectives are simultaneously optimized along with the net present value. The proposed method makes it possible to reduce the number of environmental indicators, thereby facilitating the calculation and analysis of the Pareto solutions.

1. INTRODUCTION

Energy security and environmental concerns have boosted the large-scale substitution of fossil fuels by biobased sources of energy. Nowadays, bioethanol is the world's leading transportation biofuel, with a worldwide production in 2010 of 23 billion gallons.[1] Despite this growth, there is still the open issue of assessing whether replacing fossil fuels by biofuels like bioethanol is indeed environmentally advantageous from a holistic viewpoint.[2]

The environmental assessment of bioethanol production has recently attracted increasing attention. Several mathematical models have been proposed so far to optimize the economic and environmental performance of biofuels supply chains (SCs). These approaches have mainly focused on reducing the greenhous gas (GHG) emissions of the bioethanol infrastructure. Zamboni et al. (2009)[3] formulated a biobjective optimization model that minimizes the GHG emissions associated with the future corn-based Italian bioethanol network. Recently, Zamboni et al. (2011)[4] included crop management decisions in the aforementioned model considering two objectives: total daily GHG impact and net present value (NPV). Giarola et al. (2011)[5] extended this model by adding second generation bioethanol production technologies.

Several studies[6,7] have shown that optimizing GHG emissions as a single environmental criterion can lead to solutions where such emissions are reduced at the expense of increasing other negative effects (mainly the destruction of the native tropical eco-systems and soil erosion). To avoid this, Mele et al. (2011)[8] developed a bicriteria model that maximizes the profit and minimizes the life cycle environmental impact of combined sugar/bioethanol SCs. The latter criterion was measured using two environmental indicators: the Eco-indicator 99,[9] which accounts for eleven life cycle environmental impacts pertaining to several damage categories, and the global warming potential.

The Eco-indicator 99 is an aggregated environmental metric constructed by attaching weights and normalization values to a set of single environmental indicators. The goal of normalization is to refer the original impact values to a common basis before being aggregated into a single metric. Weighting schemes rank different indicators according to their importance. They are typically defined by a panel of experts that reflect the views of the society or a group of stakeholders. The weakness of this aggregation procedure is that it uses fixed normalization and weighting parameters that may not represent the decision-makers' interests. Moreover, when used in a multiobjective optimization framework, aggregated metrics have the effect of changing the dominance structure of the problem in a manner such that some solutions may be left out of the analysis.[10]

The use of aggregated indicators in environmental multiobjective optimization (MOO) problems is a common practice in environmental engineering that was originally motivated by the numerical difficulties associated with optimizing a large number of objectives simultaneously.[11,12] An alternative approach to overcome this computational limitation consists of constructing an approximated model where the key objectives are kept and the redundant ones are omitted. So far, the elimination of objectives in environmental MOO problems has largely relied on the decision-makers' preferences, who typically select the most relevant criteria and drop the rest.

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This approach does not rely on any rigorous analysis, and for this reason it may lead to large approximation errors.

Objective reduction techniques arose in response to this situation. They allow transforming multiobjective problems with a large number of objectives into a meaningful equivalent with a reduced set of them. Ideally, the reduced representation should preserve the characteristics of the original problem, making it possible to identify the solutions of the original full space model by solving its simplified counterpart. Brockhoff and Zitzler (2006)[13] formally stated the problems of computing the smallest minimum objective subset (MOSS) that does not exceed a given maximum allowable approximation error (denoted as the δ-MOSS problem) and a minimum objective subset of size k with minimum error (k-MOSS problem). They also presented an exact and a heuristic algorithm to tackle these problems. Alternatively, Deb and Saxena (2005)[14] investigated the use of principal component analysis (PCA) to identify redundant objectives in MOO.

Despite recent advances in dimensionality reduction techniques, their use in environmental problems has been quite scarce. Sabio et al. (2011)[15] applied PCA to identify redundant life cycle assessment (LCA) metrics in the multiobjective optimization of hydrogen infrastructures, while Pozo et al. (2011)[16] proposed an improved ε-constraint method combined with PCA for dimensionality reduction and applied it to the design of petrochemical supply chains. It should be noted that despite being faster, dimensionality reduction methods based on PCA produce solutions with larger approximation errors than those based on the definition of δ-error.[13]

This work explores the application of a mixed-integer linear programming (MILP)-based objective reduction method in the design of infrastructures for ethanol production. To the best of our knowledge, this is the first contribution in the literature that addresses the optimization of these systems considering simultaneously several LCA metrics, some of which are omitted from the analysis using a rigorous approach.

The article is organized as follows. The next section describes the case study based on the design of bioethanol/sugar SCs in Argentina, which is taken as a test bed to illustrate the capabilities of our approach. The section that follows discusses concepts concerning Pareto dominance and measures of changes in the dominance structure of MOO problems resulting from removing objectives. In section 4, we briefly outline the ε-constraint method, and describe the proposed MILP that seeks to identify the subset of objectives to be omitted with minimum error. In section 5, some numerical results are presented. Finally, in section 6, the conclusions of the work are drawn.

2. PROBLEM STATEMENT: ARGENTINEAN SUGAR CANE INDUSTRY

The optimal design and planning of integrated sugar/bioethanol SCs in Argentina[8] is considered herein. We aim to determine the structure of a three-echelon SC (production−storage−market) that includes a set of plants and a set of storage facilities, where products are stored before being delivered to the final customers. The production and storage facilities can be installed in a set of subregions defined according to the administrative division of Argentina.

We consider all possible configurations of the ethanol sugar SC as well as all technological aspects associated with its performance, such as production and storage technologies, waste disposal, and transportation alternatives for raw materials and products. Five different technologies, two for sugar production and three types of distilleries, are studied. Sugar mills use sugar cane juice to produce both white and raw sugar. One type of sugar mill (T1) generates molasses as a byproduct, whereas the other one (T2) produces a secondary honey in addition to sugars. Anhydrous ethanol can be produced by fermentation and subsequent dehydration of different process streams: molasses (T3), honey (T4), and sugar cane juice (T5). The details of each technology, including the mass balance coefficients, are shown in Figure 1, where residuals, loses, and discards are omitted.

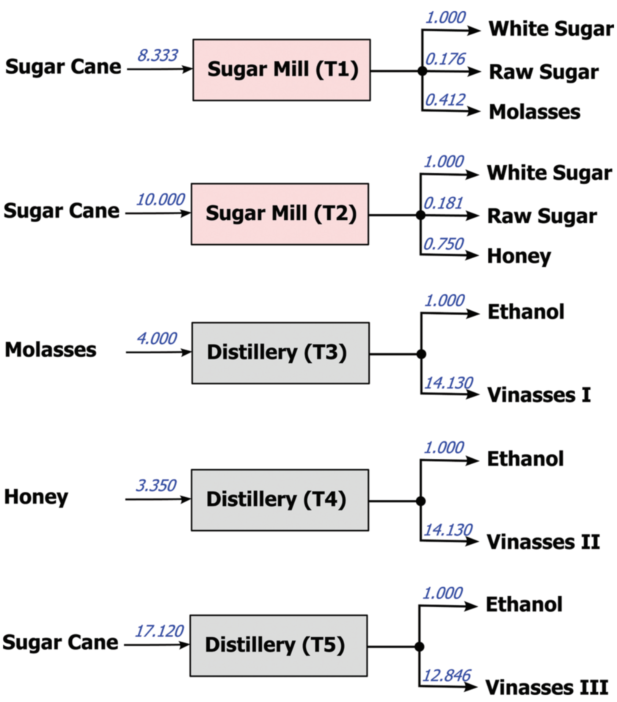

Figure 1. Set of production technologies.

Two different types of storage facilities, warehouses for liquid products (S1) and warehouses for solid materials (S2), are considered. It is assumed that materials can be transported by three different types of trucks: heavy trucks with open-box bed for sugar cane (TR1), medium trucks for sugar (TR2), and tank trucks for liquid products (TR3). Storage and transportation modes are shown in Figure 2.

Given cost and environmental data, technical details of each technology and demand to be fulfilled, we aim at determining

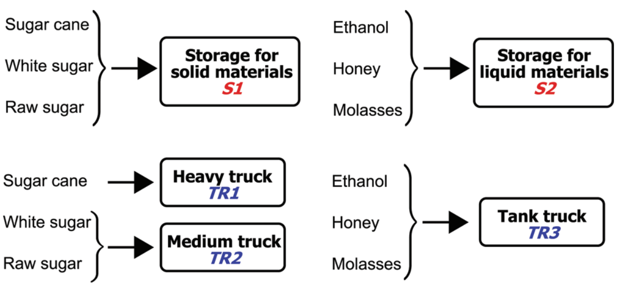

Figure 2. Set of storage and transportation technologies.

the optimal SC configuration and associated planning decisions that simultaneously optimize the economic and environmental performance of the network. An MILP formulation was introduced by the authors[8] to tackle this problem in a previous work in which the economic performance was measured *via* the NPV, whereas the environmental damage was quantified using an aggregated environmental indicator (i.e., Eco-indicator 99).

In this article, we extend this MILP by optimizing the individual impact categories considered in the Eco-indicator 99: damage to human health (DHH), damage to eco-system quality (DEQ), and damage to resources (DR), along with the global warming potential (GWP_{100}) along with the Eco-indicator 99 itself. A minimum demand satisfaction level is considered for the sugar and ethanol. Note that the Eco-indicator 99 is an aggregated metric calculated by attaching weights to a set of environmental impacts. It is clear that this aggregated metric is redundant when the individual impacts are included in the optimization, since it is expressed as a linear combination of these impacts. Despite this observation, we have decided to include such an aggregated metric in the analysis in order to discuss the limitations of using weighting schemes in LCA.

The details of the original MILP can be found in our previous publications.[8] The LCA metrics are calculated here following the same approach as in other works presented previously by the authors that combine LCA and optimization.[17−21] The inclusion of six objectives (i.e., NPV plus five LCA metrics) leads to a complex MOO problem, whose solutions are difficult to generate and interpret. We focus next on explaining how the Pareto solutions of this MILP are obtained and analyzed, which constitutes the main novelty of this work.

3. MATHEMATICAL BACKGROUND

We consider the following general multiobjective minimization problem MO(X):

$$\mathrm{MO(X)} = \min_{x \in X} (F(x) = \{f_1(x), f_2(x), \ldots f_k(x), \ldots f_O(x)\})$$

subject to

$$g_n(x) \le 0, \quad n = 1, 2, \ldots, N$$

$$h_{n'}(x) = 0, \quad n' = 1, 2, \ldots, N' \tag{1}$$

where O objective functions are optimized, N is the number of inequality constraints, and N' is the number of equality constraints. X is the search space, x is a vector of decision variables, and $F(x)$ denotes the vector of objective functions $f_k(x)$. The set of values taken by the objective functions $f_k(x)$ in the feasible solutions of MO(X) constitutes the feasible objective space Z. In the context of our problem, one of the objectives f_k represents the economic performance, whereas the others quantify a set of environmental impacts.

Figure 3 shows an illustrative example of the feasible objective space of a bicriterion problem. Solution A shows the minimum value of f_1, while solution D is better in terms of objective f_2 and worse in objective f_1. Two additional solutions (B and C) are also shown in the figure. All these solutions are Pareto-optimal or nondominated. The set of all nondominated solutions constitutes the Pareto-optimal front (thin red line edging the lower-left part of Z). Solution S_1 weakly dominates solution s_2 (i.e., $s_1 \preccurlyeq s_2$), if the following conditions hold:

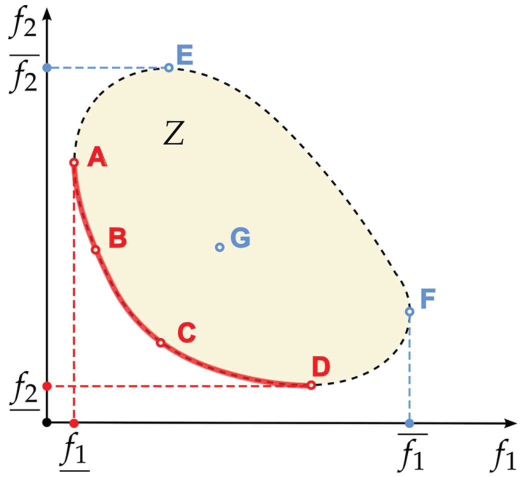

Figure 3. Hypothetical feasible objective space and Pareto optimal front for a MOO problem minimizing both objectives f_1 and f_2. Solutions A, B, C, and D are Pareto-optimal, whereas solutions E, F, and G are nonoptimal. The thin red line denotes the Pareto front.

1. Solution s_1 performs better than or equal to s_2 in all of the objectives:

$$f_k(s_1) \le f_k(s_2) \quad \forall\, k \tag{2}$$

2. Solution s_1 is strictly better than s_2 in at least one objective:

$$\exists\, k \in \{1, \ldots, M\}: \quad f_k(s_1) < f_k(s_2) \tag{3}$$

As observed, solutions E, F, and G are worst than C simultaneously in both objectives (f_1 and f_2). These solutions are called dominated or nonoptimal solutions.

The aim of any objective reduction method is to identify a subset of objectives of a MOO problem such that the error of omitting them (known as δ-error) is minimum. The concept of δ-error was first proposed by Brockhoff and Zitzler (2006).[13] We illustrate the fundamentals behind this concept using an example with three Pareto solutions and four objectives.

Figure 4 is a parallel coordinate plot,[22,23] which allows displaying large-dimensional data sets (i.e., Pareto solutions with several objectives) in a straightforward manner, providing valuable insight on their dominance structure. In the parallel coordinates plot, the x-axis represents the set of objectives, while the y-axis shows the normalized performance attained by each solution in each objective. Every line in the parallel coordinates plot represents a single solution. Note that

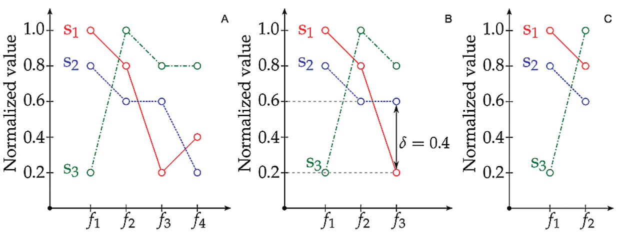

Figure 4. (a) Dominance structure of the original problem. (b) Dominance structure after removing f_4. (c) Dominance structure of the reduced set $\{f_1, f_2\}$.

solutions s_1 (solid red line), s_2 (blue dashed line), and s_3 (green dash-dotted line) are all weakly Pareto-optimal.

Further analysis of the solutions reveals that $f_k(s_2) < f_k(s_1) < f_k(s_3)$ for $k = 2$ and $k = 4$. On this basis, it is possible to remove either objective function f_2 or f_4 without changing the dominance structure of the problem. These objectives are regarded as redundant or nonessential, as omitting them does not alter the problem structure. The error of omitting one of these redundant objectives is hence zero, as the dominance structure is preserved after removing any of them (see Figure 4a,b).

There are no more nonessential objectives in this example. In fact, further reductions in the number of objectives change the dominance structure. Particularly, Figure 4c shows the reduced set of objectives $F' = \{f_1, f_2\}$. We observe that if we drop objectives f_3 and f_4, then solution s_2 dominates solution s_1 (i.e., $s_2 \preccurlyeq_{F'} s_1$), even though $f_3(s_1) < f_3(s_2)$, that is, the dominance structure is modified with respect to that of the original search space. The difference between the values of $f_3(s_1)$ and $f_3(s_2)$ can be used as a measure to quantify the change in the dominance structure. Hence, the approximation error is defined as the maximum amount that we have to subtract from a solution A that dominates another solution B in the reduced space such that A also dominates B in the original search space. For this case, this difference is equal to 0.4. This metric (referred to as δ-error) indicates to which extent the initial dominance relationship is modified after removing objectives.

Two problems of interest arise at this point. The first is to identify the minimum set of objectives that preserves the problem structure except for an error of δ. The second is to determine the minimum δ-value for a given number of objectives to be omitted. These problems were formally stated by Brockhoff and Zitzler (2006),[13] who proposed an exact and a heuristic approach to tackle them. More recently, Guillén-Gosálbez (2011)[24] introduced a rigorous MILP formulation for the efficient solution of these problems. As shown by Brockhoff and Zitzler (2006),[13] these problems are $\mathcal{NP}$-hard, that is, there is no known algorithm capable of solving them in polynomial time. In the following section we explain how these concepts and tools can be applied in the context of designing ethanol SCs with environmental concerns.

4. SOLUTION PROCEDURE

Our solution procedure comprises two steps (see Figure 5). In step one, a set of Pareto solutions of the original full space problem is generated using the ε-constraint method. In step two, a rigorous MILP-based dimensionality reduction method is applied to identify redundant objectives thereby reducing the problem complexity and facilitating the interpretation and analysis of the Pareto set. These steps can be performed iteratively until a termination criterion is satisfied (see Figure 5).

4.1. Step 1: ε-Constraint Method. MOO problems can be solved by means of several methods whose details can be found elsewhere.[11,25] In this work, we use the ε-constraint method,[26] which entails solving a set of single objective problems $SO_e(X)$ where one objective is kept in the objective function (e.g., f_1) while the rest are transferred to auxiliary constraints in which

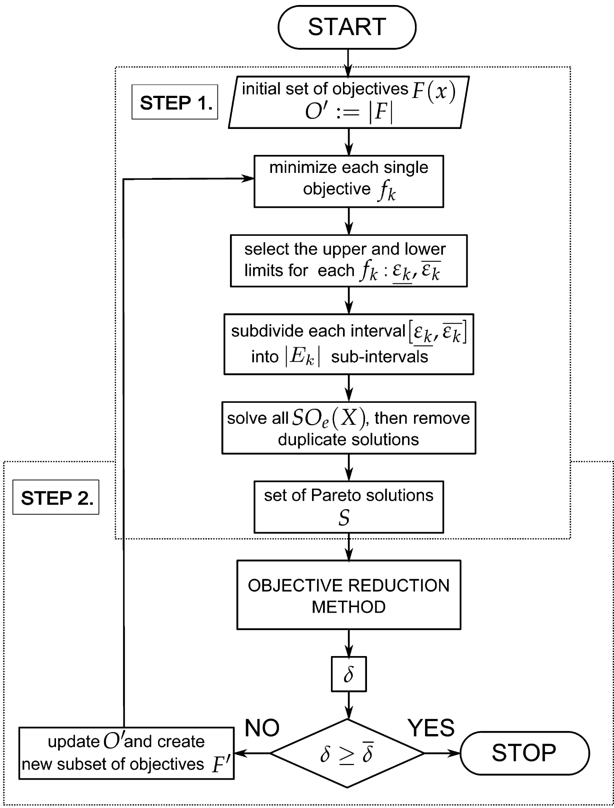

Figure 5. Solution procedure.

upper bounds are imposed on them using a set of ε-parameters ($\varepsilon_{k,e}$):

$$\begin{aligned} SO_e(X) = \; & \min_{x \in X} (f_1(x)) \\ & \text{subject to} \\ & g_n(x) \le 0, \quad n = 1, 2, ..., N \\ & h_{n'}(x) = 0, \quad n' = 1, 2, ..., N' \\ & f_k(x) \le \varepsilon_{k,e} \quad k = 2, ..., O \\ & \underline{\varepsilon_k} \le \varepsilon_{k,e} \le \overline{\varepsilon_k} \quad k = 2, ..., O \end{aligned} \tag{4}$$

Different Pareto solutions can be obtained by solving iteratively problem $SO_e(X)$ for different values of $\varepsilon_{k,e}$. In our case, we retain the NPV ($k = 1$) as main objective and transfer the environmental indicators ($k \neq 1$) to the auxiliary constraints. The lower and upper limits of each ε-parameter are obtained from the minimization of each separate environmental objective:

$$\begin{aligned} \underline{s_k} = \; & \arg \min_{x \in X} (f_k(x)), \quad k \neq 1 \\ & \text{subject to} \\ & g_n(x) \le 0, \quad n = 1, 2, ..., N \\ & h_{n'}(x) = 0, \quad n' = 1, 2, ..., N' \end{aligned} \tag{5}$$

which defines $\underline{\varepsilon_k} = f_k(\underline{s_k})$, $k \neq 1$. Furthermore, the maximum values of every objective f_k among the solutions $\underline{s_k}$ are used to define the upper bounds imposed on the epsilon parameters.

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Next, the intervals $[\underline{\varepsilon_k},\overline{\varepsilon_k}]$ are subdivided into $|E_k|$ subintervals, and model $SO_\varepsilon(X)$ is solved for each of the limits of these subintervals, generating a different Pareto solution in each run.

4.2. Step 2: Dimensionality Reduction. Step 2 entails the application of a dimensionality reduction method using the Pareto solutions generated in step 1. Two main methods for dimensionality reduction in multiobjective optimization are available: the PCA-based approach of Deb and Saxena (2005),[14] and the rigorous approach for objective reduction based on the concept of error of the approximation (Brockhoff and Zitzler (2006)[13]). The PCA method is faster, but it can lead to very large approximation errors, as was shown by Brockhoff and Zitzler (2006).[13] For this reason, we follow herein a rigorous MILP-approach based on the δ-error definition (see Guillén-Gosálbez (2011)[24]).

To this end, we proceed as follows. We first obtain a set of Pareto solutions $S = \{s_1,...,s_i,...,s_L\}$, $S \subset X$ to problem MO(X) using any MOO solution procedure. These points will be used in the MILP for objective reduction. This MILP comprises two main sets of equations, those that determine whether a solution is lost in the reduced set of objectives, and those that calculate the δ-value. We provide next an overview of this MILP. Further details can be found in the original article.[24]

We define the following notation. The binary parameter $YP_{i,i',k}$ takes the value of 1 if solution s_i is better than solution $s_{i'}$ in objective function f_k (i.e., $f_k(s_i) \le f_k(s_{i'})$) and 0 otherwise. The binary variable ZO_k is equal to 1 if objective f_k is removed from F and 0 otherwise, while binary variable $ZD_{i,i'}$ takes the value of 1 if solution $s_{i'}$ dominates solution s_i in the reduced Pareto space and 0 otherwise. The definition of the latter variable is enforced *via* the following constraints:

$$(L - \sum_k ZO_k) - L(1 - ZD_{i,i'}) \le \sum_k YP_{i',i,k}(1 - ZO_k) \le (L - \sum_k ZO_k) + L(1 - ZD_{i,i'}) \quad \forall\, i \ne i' \tag{6}$$

$$\sum_k YP_{i',i,k}(1 - ZO_k) \le (L - \sum_k ZO_k) - 1 + LZD_{i,i'} \quad \forall\, i \ne i' \tag{7}$$

The δ-error is defined as the difference between the value of objective f_k in solutions s_i and $s_{i'}$:

$$\delta_{i,i',k} = (f_k(s_{i'}) - f_k(s_i))ZO_k ZD_{i,i'} \quad \forall\, i \ne i', k \tag{8}$$

The product of binaries in eq 8 can be linearized as follows:

$$(f_k(s_{i'}) - f_k(s_i))ZOD_{i,i',k} = \delta_{i,i',k} \quad \forall\, i \ne i', k \tag{9}$$

$$ZOD_{i,i',k} \le ZO_k \quad \forall\, i \ne i', k \tag{10}$$

$$ZOD_{i,i',k} \le ZD_{i,i'} \quad \forall\, i \ne i', k \tag{11}$$

$$ZOD_{i,i',k} \ge ZO_k + ZD_{i,i'} - 1 \quad \forall\, i \ne i', k \tag{12}$$

Two MILPs can now be constructed to solve the δ-MOSS and k-MOSS problems.

For minimizing the maximum error of omitting objectives, we add a constraint imposing a bound on the maximum number of objectives removed:

$$\sum_k ZO_k = \overline{OB} \tag{13}$$

The following MILP formulation is then used to solve the k-MOSS problem:

$$\text{(MOR1)} \quad \min \max_{i,i',k} \{\delta_{i,i',k}\}$$
$$\text{subject to constraints 6–13}$$

For minimizing the number of objectives for a given error $\overline{\delta}$, we impose an upper bound on variable $\delta_{i,i',k}$ via the following inequality:

$$\delta_{i,i',k} \le \overline{\delta} \tag{14}$$

We then construct an alternative model (MOR2) for solving the δ-MOSS problem that can be expressed as follows:

$$\text{(MOR2)} \quad \max \sum_k ZO_k$$
$$\text{subject to constraints 6–12, 14}$$

The algorithm proposed for solving the multiobjective MILP for the design of ethanol infrastructures, which makes use of the rigorous MILP for dimensionality reduction, comprises the following steps: (1) Set a number of iterations of the ε-constraint method, and a threshold cut (TC). (2) Generate a set of solutions of the original MILP using the ε-constraint method. (3) Apply the MILP-based objective reduction method to the solutions generated in all the previous (and current) iterations. (4) Check the termination criterion. If it is reached, then the algorithm ends, otherwise go to step 1 and repeat steps 1 to 4 until the termination criterion is satisfied.

Remarks. (1) The MILP formulation for dimensionality reduction slightly differs from the one presented in Guillén-Gosálbez (2011).[24] Particularly, we have modified the original formulation in order to reproduce exactly the manner in which Zitzler (2006)[13] calculated the δ-error. In the original MILP model introduced in Guillén-Gosálbez (2011),[24] we omitted the error between any pair of solutions that were not Pareto optimal in the reduced space, while in the modified MILP, we consider the error between any two solutions regardless of whether they are Pareto optimal or not in the reduced space of objectives.

(2) Different termination criteria can be used in the algorithm. A termination criterion that works well is to stop when further reductions in the number of objectives cannot be obtained. Hence, a δ-error threshold is defined at the beginning of the algorithm, which is stopped when the cardinality of the set of objectives kept cannot be further reduced without surpassing the δ-error. To check this condition, we employ the MILP formulation that minimizes the minimum number of objectives for a given δ-error (MOR2).

(3) The number of iterations of the ε-constraint method can be dynamically changed during the execution of the algorithm. As iterations proceed, it will be possible to increase the number of subintervals of the ε-constraint method while still keeping the number of iterations constant, since LCA metrics will be omitted progressively from the pool of objectives.

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(4) The number of solutions used in the MILP for objective reduction will increase with the number of iterations, which will lead to larger CPU times during the phase of dimensionality reduction using the MILP formulation.

5. NUMERICAL RESULTS

The approach proposed was applied to the case study described in Mele et al. (2011)[8] (see the original publication for further details), but this time optimizing the following LCA metrics simultaneously: GWP_{100}, EI_{99}, DHH, DEQ, and DR. We implemented the ε-constraint method considering seven ε-values for each environmental metric. The model was written in GAMS[27] and solved with the MILP solver CPLEX 12.0 on a HP Compaq DC5850 desktop PC with an AMD Phenom 8600B, 2.29 GHz triple-core processor, and 2.75 Gb of RAM. This led to 16 807 iterations, 4941 of which were feasible. Only 40 solutions were finally identified after removing the repeated ones. The total CPU time spent was 58 669 s. Note that the ε-constraint algorithm is rather inefficient when applied to the original problem since several redundant metrics exist.

The structure of the maximum NPV SC (Figure 6) is quite centralized. Three sugar mills T2, one distillery T4, and three

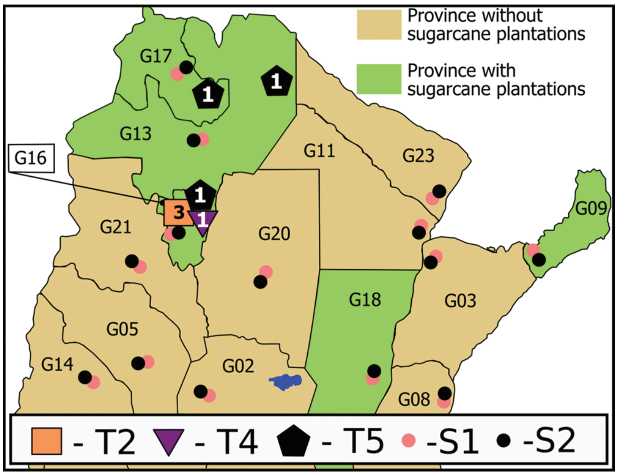

Figure 6. SC configuration for the solution with maximum NPV.

distilleries T5 are located in the northwest of Argentina. The consumption of sugar cane in this solution is 98.6%. The choice of the couple T2−T4 is due to the fact that these technologies show higher ethanol yield than that of the couple T1−T3.

In the minimum GWP_{100} solution (Figure 7), 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 established in the five provinces that have sugar cane plantations. This solution consumes all the sugar cane available. This configuration decreases the CO_2 emissions, since sugar cane cultivation has a negative value of GWP_{100}.[8] The choice of the tandem T1−T3 is motivated by their lower GWP_{100} as compared with T2−T4.

The SC structure with minimum EI_{99} (Figure 8) is also the one with minimum DHH, DEQ, and DR values. The network shows similar topology as the minimum GWP_{100} solution. However, instead of T1 and T3, it operates with T2 and T4 as occurred in the solution with maximum NPV. The choice of T2−T4 is explained by their lower EI_{99}, DHH, DEQ, and DR

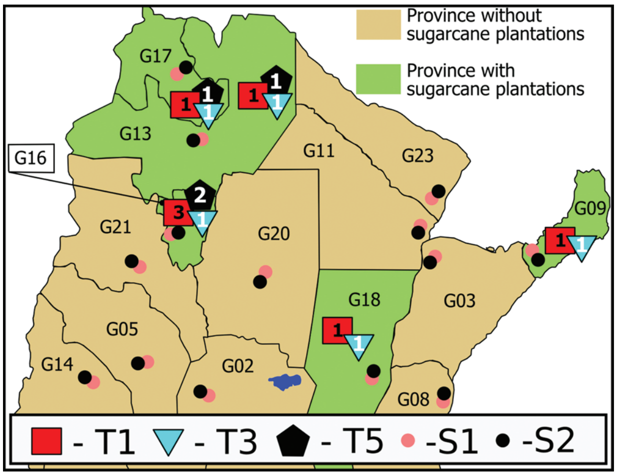

Figure 7. SC configuration for the solution with minimum GWP_{100}.

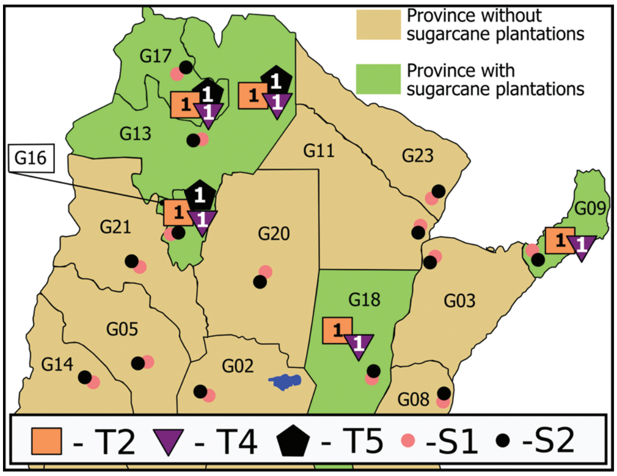

Figure 8. SC configuration for the solution with minimum EI_{99}, DHH, DEQ, and DR.

impacts. All the production, storage, and transportation activities considered in the model show positive values of these four environmental metrics. Hence, minimizing these environmental metrics produces solutions in which the production, storage, and transportation tasks are reduced. Note that due to the demand satisfaction constraints, the model is forced to cover a minimum demand of sugar and ethanol. Since the pair T2 and T4 cannot produce as much ethanol as white sugar, the model decides to open three T5 distilleries to produce the amount of ethanol required to attain a demand satisfaction of 30%.

The Pareto-optimal solutions were next normalized prior to solving the MILP for dimensionality reduction. The NPV values were normalized as follows:

$$nf_k(s_i) = \frac{\overline{f_k} - f_k(s_i)}{\overline{f_k} - \underline{f_k}} \quad \forall\ i,\ k = 1 \tag{15}$$

where $\overline{f_k}$ and $\underline{f_k}$ denote the maximum and minimum values of objective f_k among all the Pareto solutions. The normalized

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values of the environmental indicators were calculated as follows:

$$nf_k(s_i) = \frac{f_k(s_i) - \underline{f_k}}{\overline{f_k} - \underline{f_k}} \quad \forall\ i, k \neq 1 \tag{16}$$

Figure 9 is a parallel coordinates plot that depicts the normalized Pareto points obtained following the above

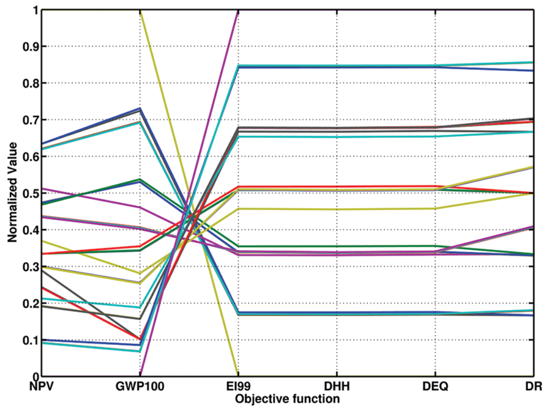

Figure 9. Parallel coordinate plot.

commented procedure. This plot suggests that objectives EI_{99}, DHH, and DEQ are redundant, since they all behave in a similar manner in all the Pareto-optimal solutions. Impact DR is also somehow redundant with these metrics but to a lesser extent.

We next applied the proposed MILP-based approach recursively. Specifically, the MILP was first ran for a given number of objectives to be removed forcing the model to keep the NPV, and the solution (i.e., combination of objectives) identified in this first iteration was eliminated using an integer cut.[28]

We repeated this procedure until the MILP turned out to be infeasible. The results are presented in Tables 1−4, in which all

Table 1. δ-Error for All Combinations of NPV and One of the Environmental Metrics

reduced subset	δ-Error × 100
{NPV, GWP_{100}}	100.00
{NPV, EI_{99}}	15.20
{NPV, DHH}	15.20
{NPV, DEQ}	15.20
{NPV, DR}	15.20

possible combinations of 2, 3, 4, and 5 objectives are displayed along with the corresponding approximation errors. As seen, four LCA metrics are required to fully preserve the dominance structure: NPV, GWP_{100}, DR, and then either EI_{99}, or DEQ, or DHH. Further reductions in the number of objectives change the dominance structure. Note, however, that there are combinations of 3 objectives with very small δ-values. All of them contain NPV and GWP_{100}, and differ only in the third objective, which is either the EI_{99}, DEQ, DHH, or DR. Among the combinations of three metrics, the subset NPV, GWP_{100}, DR has the smallest error. The subsets with NPV, GWP_{100} and objectives EI_{99}, DEQ, or DHH show similar δ-values, since these three last objectives are all redundant. As seen, there are

Table 2. δ-Error for All Combinations of NPV and Two of the Environmental Metrics

reduced subset	δ-Error × 100
{NPV, GWP_{100}, EI_{99} }	7.49
{NPV, GWP_{100}, DHH }	7.82
{NPV, GWP_{100}, DEQ }	7.65
{NPV, GWP_{100}, DR }	0.15
{NPV, EI_{99}, DHH }	15.20
{NPV, EI_{99}, DEQ }	15.20
{NPV, EI_{99}, DR }	15.20
{NPV, DHH, DEQ }	15.20
{NPV, DHH, DR }	15.20
{NPV, DEQ, DR }	15.20

Table 3. δ-Error for All Combinations of NPV and Three of the Environmental Metrics

reduced subset	δ-Error × 100
{NPV, GWP_{100}, EI_{99}, DHH }	7.49
{NPV, GWP_{100}, EI_{99}, DEQ }	7.49
{NPV, GWP_{100}, EI_{99}, DR }	0
{NPV, GWP_{100}, DHH, DEQ }	7.65
{NPV, GWP_{100}, DHH, DR }	0
{NPV, GWP_{100}, DEQ, DR }	0
{NPV, EI_{99}, DHH, DEQ }	15.20
{NPV, EI_{99}, DHH, DR }	15.20
{NPV, EI_{99}, DEQ, DR }	15.20
{NPV, DHH, DEQ, DR }	15.20

Table 4. δ-Error for All Combinations of NPV and Four of the Environmental Metrics

reduced subset	δ-Error × 100
{NPV, GWP_{100}, EI_{99}, DHH, DEQ }	7.49
{NPV, GWP_{100}, EI_{99}, DHH, DR }	0
{NPV, GWP_{100},EI_{99}, DEQ, DR }	0
{NPV, GWP_{100}, DHH, DEQ, DR }	0
{NPV, EI_{99}, DHH, DEQ, DR }	15.20

three main clusters of environmental objectives: (1) GWP, (2) EI_{99}, DEQ and DHH, and (3) DR. The latter two are closer between them than with objective GWP_{100}. Note that we could also apply a statistical approach such as PCA to identify these clusters. This method, however, does not provide any information on the error of the approximation obtained after removing redundant objectives.

Figure 10 shows the projections of the points generated using the ε-constraint method onto the 2-D subspaces NPV vs GWP_{100}, NPV vs DEQ, NPV vs DHH, NPV vs DR, and NPV vs EI_{99}. Note that, according to the normalization performed using eq 15, the NPV values decrease as we get close to 1. In contrast, the environmental impacts are reduced as their normalized values approach to zero. As seen, as the NPV grows, the GWP_{100} decreases. This is because larger profits are attained by increasing the cultivation of sugar cane, which adsorbs large amounts of CO_2, thereby decreasing the GHG emissions of the whole bioethanol network. The remaining environmental metrics behave in an opposite manner, that is, they increase with the NPV value. This is because, as shown in Mele et al. (2011),[8] the production of bioethanol from sugar cane leads to positive overall LCA impacts in these categories. As seen, the points resulting from the minimization of those metrics belonging to cluster (2) overlap in Figure 10, whereas the

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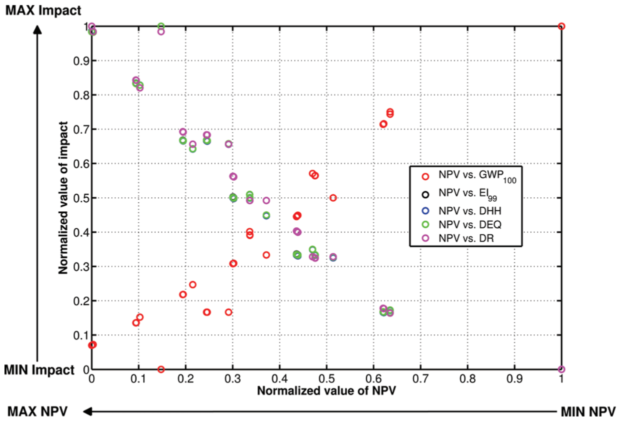

Figure 10. Bicriteria projections of the normalized values of the environmental impacts and NPV.

points denoting DR values are quite close to them. As observed, there is no single environmental metric capable of keeping the problem structure. Note that for all the combinations of NPV and an LCA metric it happens that there are points that lie below the corresponding 2-D Pareto front. Hence, regardless of the LCA metric of choice, it will be impossible to generate all the Pareto points with one single LCA metric, since many solutions will be lost after being projected onto a 2-D subspace.

Figures 11−14 show the impacts corresponding to the cultivation of sugar cane, production of sugars and ethanol, and

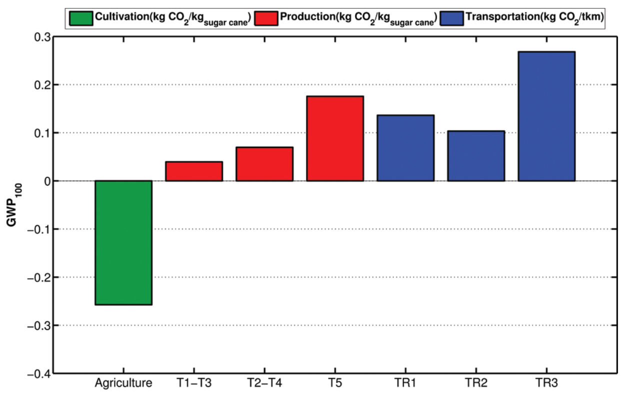

Figure 11. GWP_{100} values for different SC activities. Impact of agriculture is given per kg of sugar cane cultivated. Impact of production is given per kg of sugar cane converted. Impact of transportation is given per ton of material transported 1 km.

transportation of products and feedstocks. As discussed previously, in the case of GWP_{100}, the production and transportation tasks cause the largest impact, while sugar cane plantations show negative impact values. In contrast, all the SC activities lead to positive impacts in the remaining LCA categories. Metric DR differs from EI_{99}, DEQ, and DHH, in that it shows larger impacts in transportation and lower impacts in sugar cane cultivation.

After identifying the redundant metrics, we can run again the ε-constraint method eliminating nonessential objectives from the search. Information on how the objectives can be grouped into clusters is rather valuable as it allows decision-makers concentrating their efforts on measuring only a reduced

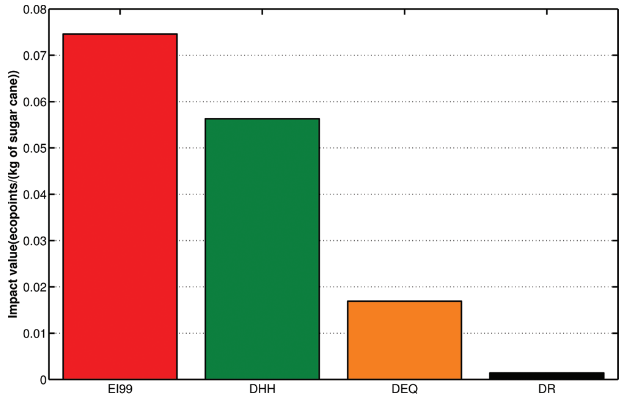

Figure 12. Impact of agriculture in terms of EI_{99}, DHH, DEQ, and DR.

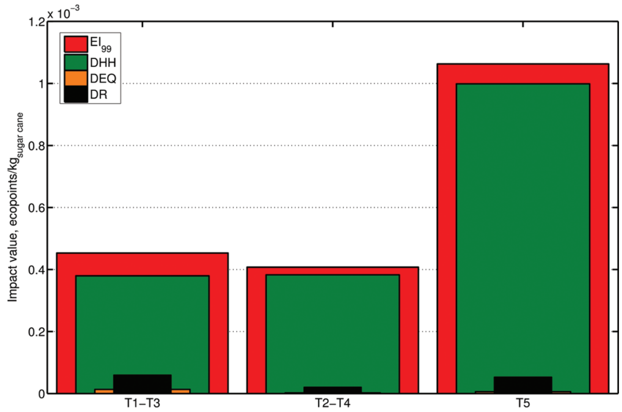

Figure 13. Impact of the different production technologies in terms of EI_{99}, DHH, DEQ, and DR. Impact values are given per kg of sugar cane converted.

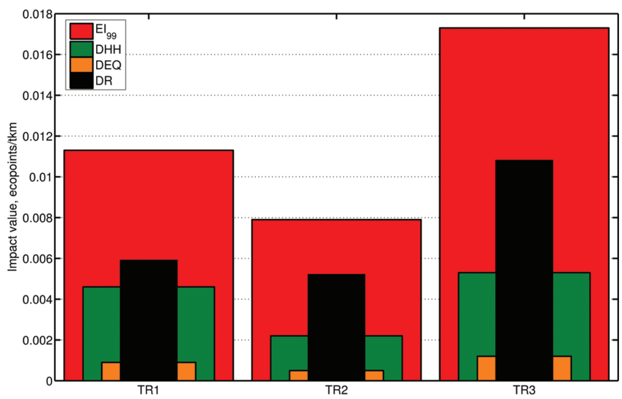

Figure 14. Impact of the different transportation technologies in terms of EI_{99}, DHH, DEQ, and DR. Impact values are given per ton of material transported for 1 km.

number of impacts, which leads to significant economic and time savings regarding data collection and computational time.

We should note that in practice there might be sources of uncertainty affecting the LCA calculations.[29−32] Even in these cases, it is still possible to use the MILP-method for dimensionality reduction by defining the LCA metrics as stochastic variables rather than as nominal values, and then

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applying the MILP to identify redundancies between these stochastic LCA metrics.

6. CONCLUSIONS

In this work, we investigated the existence of redundant LCA metrics in the multiobjective design of integrated bioethanol/sugar SCs in Argentina. To this end, we applied a rigorous MILP-based dimensionality reduction method that minimizes the error of the approximation obtained after omitting redundant objectives. Numerical results showed that the Eco-indicator 99, damage to human health, and damage to eco-system quality (and, to a lesser extent, damage to depletion of resources) behave similarly (i.e., they are somehow redundant in our problem). This makes it possible to perform the optimization in a reduced domain while still obtaining high quality results. Our approach facilitates the calculation and analysis of the Pareto solutions, providing valuable insight on the trade-offs between the objectives considered in the analysis and guiding decision-makers toward the adoption of more sustainable alternatives.

■ AUTHOR INFORMATION

Corresponding Author

*E-mail: gonzalo.guillen@urv.cat.

Notes

The authors declare no competing financial interest.

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■ NOTATION

GHG = greenhouse gas
GWP_{100} = global warming potential over a 100-year time horizon
DEQ = damage to eco-system quality
DHH = damage to human health
DR = damage to resourses
EI_{99} = eco-indicator 99
LCA = life cycle assessment
MILP = mixed-integer linear programming
MOO = multiobjective optimization
MO(X) = multiobjective model
MOSS = minimum objective subset
PCA = principal component analysis
SC = supply chain
$SO_e(X)$ = single objective model
X = feasible decision variables space
Z = feasible objective space

Sets/indices

E_k = set of ε-values indexed by e for objective function k
F = set of objective functions indexed by k
F' = reduced subset of objective functions
S = set of Pareto solutions indexed by i

Parameters

$\overline{f_k}$ = maximum value of objective f_k
$\underline{f_k}$ = minimum value of objective f_k
L = number of objectives in S
$n\,f_k$ = normalized value of objective f_k
O = number of objective functions in F
$\underline{O'}$ = number of objective functions in subset F'
$\overline{OB}$ = maximum number of objectives removed
$\underline{s_k}$ = solution in which objective f_k attains its minimum value
TC = termination criterion
$YP_{i,i',k}$ = binary parameter that takes the value of 1 if solution s_i is better than solution $s_{i'}$ in objective function f_k and 0 otherwise

Variables

OB = number of objectives removed
$ZD_{i,i'}$ = binary variable (1 if solution $s_{i'}$ dominates solution s_i in the reduced Pareto space and 0 otherwise)
ZO_k = binary variable (1 if objective f_k is removed from F and 0 otherwise)
$ZOD_{k,i,i'}$ = auxiliary binary variable
$d_{i,i',k}$ = difference between the value of objective f_k in solutions s_i and $s_{i'}$

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9.5 Dimensionality reduction applied to the simultaneous optimization of the economic and life cycle environmental performance of supply chains

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Dimensionality reduction applied to the simultaneous optimization of the economic and life cycle environmental performance of supply chains

Andrei Kostin[a], Gonzalo Guillén-Gosálbez[a,*], Laureano Jiménez[a]

[a]*Departament d'Enginyeria Química (EQ), Escola Tècnica Superior d'Enginyeria Química (ETSEQ), Universitat Rovira i Virgili (URV), Campus Sescelades, Avinguda Països Catalans, 26, 43007 Tarragona, Spain*

Abstract

The design and planning of sustainable supply chains has primarily focused on minimizing greenhouse gas emissions (GHG). Such one-sided environmental assessment may lead to supply chain configurations in which GHG emissions are decreased at the expense of increasing other life cycle damages caused by the target network. Unfortunately, minimizing several environmental objectives simultaneously following a holistic approach leads to hard optimization problems. While it is possible to merge single environmental objectives into aggregated indicators, this has the disadvantage of modifying the original dominance structure of the problem in a manner such that some optimal solutions might be left out of the analysis. In this paper, we present a rigorous computational framework for solving complex multi-objective optimization (MOO) problems encountered in environmental engineering. Our strategy combines the traditional ε-constraint method with an objective reduction algorithm. The latter allows identifying redundant objectives that can be omitted while still preserving the original dominance structure, thereby reducing the associated computational complexity. The advantages of our method are demonstrated by means of two case studies that address the multi-objective optimization of supply chains that produce bioethanol and hydrogen for vehicle use, respectively.

Keywords: Sustainable supply chains, Life cycle assessment, Mixed integer linear programming, Multi-objective optimization, Dimensionality reduction

1. Introduction

Over the past decade, the minimization of the environmental impact of supply chains (SCs) has received much attention in both academia and industry. Such interest has been mainly motivated by the

*Correspondence concerning this article should be addressed to Gonzalo Guillén-Gosálbez at gonzalo.guillen@urv.cat
Email addresses: andrey.kostin@urv.cat (Andrei Kostin), gonzalo.guillen@urv.cat (Gonzalo Guillén-Gosálbez), laureano.jimenez@urv.cat (Laureano Jiménez)

growing consumer demand for "greener" products along with tighter environmental protection laws. Following this trend, major companies such as Johnson & Johnson, Intel, and General Electric have rearranged their processes and services to minimize their negative influence on the environment, and many more are planning to follow the same path.

The incorporation of environmental aspects in supply chain management (SCM) has led to the concept of green supply chain management (GrSCM), whose key idea is to integrate environmental decisions into elementary SC phases including product design, material souring and selection, manufacturing processes, delivery of final products to customers, and end-of-life management of products after their useful life (Hervani et al., 2005; Srivastava, 2007). In his extensive review, Srivastava (2007) recognized two main approaches in the area of GrSCM: empirical studies and mathematical modeling techniques. Among mathematical modeling tools, multi-objective optimization (MOO) has gained wider interest in the research community, as it offers the possibility of balancing economic and environmental issues in a systematic manner.

The overwhelming majority of MOO models applied in SCM minimize the amount of emitted GHGs, mainly because carbon emissions are regulated by the European Union Emission Trading Scheme (EU ETS), the world's largest emissions trading mechanism, whose main purpose is to mitigate climate change.

Hugo et al. (2005) presented a bi-objective model for the optimal design of hydrogen SCs that maximizes the net present value (NPV) and minimizes the GHG emissions. Zamboni et al. (2011) proposed a bi-objective model for optimizing biofuel networks that minimizes the amount of GHG. Giarola et al. (2011) and Giarola et al. (2012) proposed bi-objective models for the design of bioethanol SCs in Italy that minimize the emitted CO_2. More recently, Akgul et al. (2012) adopted a similar approach for optimizing bioethanol SCs in the UK.

Some authors have claimed that optimizing GHG emissions as unique criterion can lead to solutions where this metric is reduced at the expense of increasing other negative environmental effects (Scharlemann and Laurance, 2008; Vries et al., 2010; Cooper and Sehlke, 2012). A possible manner to avoid this consists of optimizing aggregated environmental metrics obtained by attaching weights to single impact indicators (see Huppes and van Oers, 2011). Particularly, aggregated metrics based on life cycle assessment (LCA) principles (Curran, 2006) have gained wider interest in the recent past as they allow assessing the environmental impact considering all the stages in the life cycle of the process. The Eco-indicator is one of these LCA metrics (Goedkoop and Spriensma, 1999) that has been widely used in SCM. Guillén-Gosálbez and Grossmann (2009) used the Eco-indicator 99 in the design of petrochemical SCs and hydrogen SCs for vehicle use (Guillén-Gosálbez et al., 2010). The same metric was employed by Duque et al. (2010) and Pinto-Varela et al. (2011) for optimizing industrial networks in Portugal. Neto et al. (2008) applied another aggregated metric that weights seven single impacts for optimizing paper logistic networks, while Bojarski et al. (2009) applied the IMPACT2002+ in the optimization of SCs.

The computation of aggregated metrics involves two main steps: normalization and weighting. The aim of normalization is to refer the original impact values to a common basis before being aggregated into a single metric. Weighting procedures range different indicators according to some political targets. They are typically defined by a panel of experts that reflect the views of the society or a group of stakeholders. The weakness of the aggregation procedure is that it uses fixed normalization and weighting parameters that may not represent the decision-makers' interests. Moreover, when used in an MOO framework, aggregated metrics may change the dominance structure of the problem in a manner such that some solutions may be left out of the analysis (Brockhoff and Zitzler, 2010).

The use of aggregated indicators in environmental MOO problems is a common practice in environmental engineering that was originally motivated by the numerical difficulties associated with optimizing a large number of objectives simultaneously (Ehrgott, 2000). An alternative approach that avoids the use of aggregated metrics consists of optimizing approximated models that contain only some key environmental indicators. Objective reduction techniques can be used in this context for identifying redundant objectives that can be omitted, thereby generating a meaningful equivalent with a reduced subset of them. Ideally, the reduced representation should preserve the characteristics of the original problem, making it possible to identify the solutions of the original full space model by solving its simplified counterpart. Brockhoff and Zitzler (2006) were the first to formally state the problem of computing a minimum objective subset (MOSS) without losing information (denoted as the δ-MOSS problem) and a minimum objective subset of size k with minimum error (k-MOSS problem). They presented an exact and a heuristic algorithm to tackle these problems. Alternatively, Deb and Saxena (2005) investigated the use of principal component analysis (PCA) to identify redundant objectives in MOO. Recently, Thoai (2012) proposed an approach to reduce the number of criteria and the dimension of a linear MOO problem using the concept of so-called representative and extreme criteria, while López Jaimes et al. (2008) introduced two new algorithms to reduce the number of objectives in MOO based on a feature selection technique.

Despite recent advances in dimensionality reduction techniques, their use in environmental problems has been quite scarce. Sabio et al. (2012) applied PCA to identify redundant LCA metrics in the multi-objective optimization of hydrogen infrastructures, while Pozo et al. (2011) proposed an improved ϵ-

constraint method that made used of PCA for reducing the dimensionality of the problem and applied it to the design of petrochemical supply chains. Despite being faster, dimensionality reduction methods based on PCA produce solutions with larger approximation errors than those based on the definition of δ-error (Brockhoff and Zitzler, 2006).

In this work, we propose to integrate the classical ε-constraint method with a rigorous MILP for dimensionality reduction in order to expedite the search for Pareto optimal solutions, placing a strong emphasis on environmental applications. From numerical experiments we conclude that the enhanced ε-constraint method outperforms the standalone one in terms of quality of the Pareto set produced and time spent in its calculation.

The article is organized as follows. The problem under study is formally defined in the next section. The modeling framework and solution procedure follow. Some numerical results are presented in section 4, while the conclusions of the work are drawn in section 5.

2. Problem statement

To formally state the problem of interest, we consider a generic three-echelon SC (production-storage-market) like the one depicted in Figure 1. This network includes a set of production and storage facilities, along with a set of final markets whose demand must be fulfilled. The facilities can be installed in a set of potential locations in which the overall region of interest is divided. Terrestrial transportation between sub-regions is performed using either trucks, railroad, or pipelines. In addition, different types of cargo ships can provide maritime transportation.

The problem can then be stated as follows:

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

The goal is to determine the configuration of a three-echelon network and associated planning decisions that maximize the economic performance for a given time horizon and minimize the environmental impact (which is measured over the entire life cycle of the process using LCA principles). Decisions to be made include the number, type and location of the technologies selected, the capacity of production plants and warehouses to be set up in each sub-region, their capacity expansion policy for a given forecast of prices and demand over the planning horizon, the transportation links and transportation modes of the network, and the production rates and internal flows of feed stocks, wastes and final products. In this work, without loss of generality, we focus on two design problems that follow this general pattern: the design of supply chains for ethanol and sugar production and the strategic planning of hydrogen supply chains for vehicle use (see Kostin et al., 2012; Sabio et al., 2012, for further details).

3. Solution procedure

The design problem is formulated in mathematical terms as a multi-objective mixed-integer linear program (MILP), where continuous variables model capacities, transportation flows and economic and environmental indicators, while binary variables denote the establishment of production and storage facilities. A key feature of these MILPs as applied to the environmental conscious design and planning of supply chains is that they include several environmental objectives that are calculated following LCA principles. In this work we will focus on how to solve these models efficiently. Details on the equations and variables of these MILPs can be found elsewhere (Guillén-Gosálbez and Grossmann, 2010; Kostin et al., 2012; Mele et al., 2011; Sabio et al., 2012).

For simplicity, we consider from now on the following multi-objective optimization (MOO) formulation:

$$\begin{aligned} MO(X) = & \min_{x \in X} (F_0(x)) \\ \text{s.t. } & g_n(x) \leq 0, \quad n = 1, 2, \ldots, N \\ & h_{n'}(x) = 0, \quad n' = 1, 2, \ldots, N' \end{aligned} \tag{1}$$

where $X \neq \emptyset$ is the feasible search space, and x is the vector of decision variables. $F_0(x) = \{f_1, \ldots, f_K\}$ is a given set of objective functions $f_i(x)$ $(i = 1, \ldots, K)$. N is the number of inequality constraints, whereas N' denotes the number of equality constraints. The Pareto set of solutions of problem $MO(X)$ is denoted by $S = \{s_1, \ldots, s_J\}$. The Pareto-optimal solutions s_p $(p = 1, \ldots, J)$ can be generated by means of several solution methods whose details can be found elsewhere (see Ehrgott, 2000; Deb, 2001). In this work, without loss of generality, we will make use of the ε-constraint method (Haimes et al., 1971).

Environmental engineering problems typically lead to complex MOO models with a large number of objectives, which are required to assess the environmental performance holistically. The pivotal idea of our approach is to perform the optimization task of model MOO in the space of a reduced number of objectives that capture the main features of the problem, thereby reducing the associated complexity. We proposed to identify this set using a rigorous dimensionality reduction technique based on an MILP formulation presented by the authors in a previous work (Guillén-Gosálbez, 2011).

The approach presented comprises three main steps. First, a set of Pareto solutions of model MOO is generated. A rigorous dimensionality reduction method is next applied taking these solutions as input data in order to identify redundant objectives that can be omitted without losing information. The multi-objective solution method is then executed in the reduced space of objectives, and the overall procedure is repeated until no further reductions in the number of objectives are possible. In this work we assume, without loss of generality, that the Pareto solutions are calculated using the ε-constraint method. Note, however, that any other MOO algorithm could be employed instead. Hence, the main steps of the algorithm are the following.

Step 1: Generate an initial set of Pareto-optimal solutions via the ε-constraint method. The ε-constraint method entails solving a set of single objective problems $SO_e(X)$ $(e = 1, \ldots, L)$ where one objective is retained in the objective function (*e.g.*, f_1) while the rest are transferred to auxiliary inequality constraints that impose upper bounds on them :

$$\begin{aligned} SO_e(X) = & \min_{x \in X} (f_1(x)) \\ \text{s.t. } & g_n(x) \leq 0, \quad n = 1, 2, \ldots, N \\ & h_{n'}(x) = 0, \quad n' = 1, 2, \ldots, N' \\ & f_i(x) \leq \varepsilon_{i,e} \quad k = 2, \ldots, O \\ & \underline{\varepsilon_i} \leq \varepsilon_{i,e} \leq \overline{\varepsilon_i} \quad i = 2, \ldots, O \end{aligned} \tag{2}$$

Different Pareto solutions can be obtained by solving iteratively problem $SO_e(X)$ for different values of $\varepsilon_{i,e}$. In our case, we retain the NPV $(i = 1)$ as main objective and transfer the environmental indicators $(i \neq 1)$ with the auxiliary constraints. The lower limit of each ε-parameter is obtained from the optimization of each separate environmental objective:

$$\begin{aligned} \underline{s_i} = & \arg \min_{x \in X} (f_i(x)), \ i \neq 1 \\ \text{s.t } & g_n(x) \leq 0, \quad n = 1, 2, \ldots, N \\ & h_{n'}(x) = 0, \quad n' = 1, 2, \ldots, N' \end{aligned} \tag{3}$$

which defines $\underline{\varepsilon_i} = f_i(\underline{s_i})$, $i \neq 1$. On the other hand, the upper limits $\overline{\varepsilon_i}$ are given by the maximum values of every objective f_i among the solutions $\underline{s_i}$.

Next, the intervals $[\underline{\varepsilon_i}, \overline{\varepsilon_i}]$ are subdivided into $L-1$ sub-intervals, and model $SO_e(X)$ is solved for each of the limits of these sub-intervals, generating a different Pareto solution in each run.

For generating the initial set of Pareto solutions taken as a basis in the dimensionality reduction method, we propose a heuristic approach that solves a set of bi-criteria optimization problems. In essence, we produce the initial solutions by solving a set of bi-criteria problems corresponding to all possible combinations of objectives (excluding those objectives whose optimization produces the same solution). Note that the solutions generated in the reduced bi-objective space are all guaranteed to be weakly Pareto optimal in the original search space. Furthermore, while it is possible to execute the ε-constraint method considering a larger set of objectives, this typically leads to more infeasible and/or repeated solutions than in the case of solving the bi-criteria models. This is because correlations between objectives are typically neglected when defining the ε-limits imposed on the objectives that are transferred to the auxiliary constraints.

Step 2: Apply the dimensionality reduction method. Next, a rigorous MILP-based dimensionality reduction method is applied to the set of Pareto solutions generated in step 1. This method aims to identify a subset of objectives that can be omitted while keeping the problem structure to the extent possible. To quantify the change in the dominance structure that occurs after removing objectives, we make use of the δ-error metric originally proposed by Brockhoff and Zitzler (2006).

To acquaint the reader with this concept, we next provide an illustrative example with three Pareto-optimal solutions and four objectives. Figure 2a is a parallel coordinate plot (Inselberg, 1985; Wegman, 1990), which allows displaying large-dimensional data sets (i.e., Pareto-optimal solutions with more than three objectives) in a straightforward manner, providing valuable insight on their dominance structure. In the parallel coordinates plot, the x-axis represents the set of objectives, while the y-axis shows the normalized objective values attained by each solution in every criterion. Every line in the parallel coordinates plot represents a single solution.

As seen in Figure 2a , objectives 2 and 4 lead to the same ranking of solutions, that is, $f_i(s_2) < f_i(s_1) < f_i(s_3)$ for $i = 2$ and $i = 4$. Based on this, it is possible to remove either objective function f_2 or f_4 without changing the dominance structure of the problem. These objectives are regarded as redundant or nonessential, as omitting any of them does not alter the problem structure. The error of omitting one of these redundant objectives is hence zero, as the dominance structure is preserved after removing any of them (see Figures 2a and 2b).

In this example, there are no more non-essential objectives and further reductions in the number of objectives change the dominance structure. Particularly, Figure 2c depicts the reduced set of objectives $F = \{f_1, f_2\}$. As shown, if we drop objective f_3, then solution s_2 dominates solution s_1 (i.e., $s_2 \preccurlyeq_F s_1$), even though $f_3(s_1) < f_3(s_2)$, that is, this does not happen in the original search space. The difference between the value of $f_3(s_1)$ and $f_3(s_2)$ can be used as a measure to quantify the change in the dominance structure. Hence, the maximum amount that we have to subtract from a solution that dominates another one in the reduced space such that it also dominates it in the original search space is employed to measure the approximation error. For this case, this difference is equal to 0.4. This metric (referred to as δ-error) indicates to which extent the initial dominance relationship is modified after removing objectives. The goal of our analysis is therefore to identify objectives that lead to the minimum approximation error when they are omitted from the model. To this end, in this work, we make use of the MILP proposed by (Guillén-Gosálbez, 2011) for dimensionality reduction. We next outline the main features of this approach.

Assume the existence of a set of Pareto solutions $S = \{s_1 \ldots, s_p, \ldots, s_J\}$, $S \subset X$ of problem $MO(X)$ that is generated using any MOO solution procedure. We define the following notation. The binary parameter $YP_{p,p',i}$ takes the value of 1 if solution s_p is better than solution $s_{p'}$ in objective function f_i (i.e., $f_i(s_p) \leq f_i(s_{p'})$) and 0 otherwise. The binary variable ZO_i is equal to 1 if objective f_i is removed from F_0 and 0 otherwise, while binary variable $ZD_{p,p'}$ takes the value of 1 if solution $s_{p'}$ dominates solution s_p in the reduced Pareto space and 0 otherwise.

Figure 3 clarifies the notation used in the article. In this example, two functions f_1 and f_4 are removed from the original space, that is $ZO_1 = 1$ and $ZO_4 = 1$. As shown, solution s_1 dominates solution s_2 in the reduced space ($ZD_{2,1} = 1$). The definition of the variable $ZD_{p,p'}$ is enforced via the following constraints:

$$(K - \sum_i ZO_i) - L(1 - ZD_{p,p'}) \leq \sum_i YP_{p',p,i}(1 - ZO_i) \leq (K - \sum_i ZO_i) + K\,(1 - ZD_{p,p'}) \quad \forall p \neq p' \quad (4)$$

$$\sum_i YP_{p',p,i}(1 - ZO_i) \leq (K - \sum_i ZO_i) - 1 + K\,ZD_{p,p'} \quad \forall p \neq p' \quad (5)$$

K denotes the number of objectives in the original space, that is $|F_0|$. Therefore, if s_p dominates $s_{p'}$, then $YP_{p',p}$ will be equal to 1 for all the objectives for which $ZO_i = 0$, and the summation of $YP_{p',p}$ will equal the number of objectives kept in the reduced space. Constraint 5 guarantees that this will hold if $ZD_{p,p'} = 1$. On the other hand, if solution $s_{p'}$ does not dominate s_p, then there will be objectives in which s_p will be better than $s_{p'}$ and others in which the opposite will hold. Consequently, the term$YP_{p',p,i}(1 - ZO_i)$ will be necessarily lower than the cardinality of the set of objectives kept, and equation 5 will force the binary variable $ZD_{p,p'}$ to take the value of 0.

The following constraint specifies the total number of omitted objectives (OB):

$$\sum_i ZO_i = OB \tag{6}$$

The δ-error is defined as the difference between the value of objective f_i in solutions s_p and $s_{p'}$:

$$\delta_{p,p',i} = \left(f_i(s_{p'}) - f_i(s_p)\right) ZOD_{p,p',i} \quad \forall i, p \neq p' \tag{7}$$

where $ZOD_{p,p',i}$ is defined via the following constraints:

$$ZOD_{p,p',i} \leq ZO_i \quad \forall i, p \neq p' \tag{8}$$

$$ZOD_{p,p',i} \leq ZD_{p,p'} \quad \forall i, p \neq p' \tag{9}$$

$$ZOD_{p,p',i} \geq ZO_i + ZD_{p,p'} - 1 \quad \forall i, p \neq p' \tag{10}$$

As observed, the value of $\delta_{p,p',i}$ is determined only for those solutions s_p dominated by at least another solution $s_{p'}$ in the reduced space of objectives, and only for the omitted objectives $f_i \notin F$. On the other hand, constraint 7 forces variable $\delta_{p,p',i}$ to take a zero value when s_p is Pareto optimal in the reduced space and f_i is a non-omitted objective. Note that in the latter case variable $ZOD_{p,p',i}$ will take a zero value, making $\delta_{p,p',i}$ equal to zero.

Based on these constraints, we can now derive MILP to solve the δ-MOSS problem (i.e. identify the objectives that lead to the minimum δ-error):

$$(\delta\text{-MOSS}) \quad \min \max_{p,p',i} \{\delta_{p,p',i}\}$$
$$\text{s.t. constraints 4–10}$$

For minimizing the number of objectives for a given error $\overline{\delta}$, we impose an upper bound on variable $\delta_{i,i',k}$ via the following inequality:

$$\delta_{p,p',i} \leq \overline{\delta} \tag{11}$$

To calculate the smallest possible set of objectives that preserves the original dominance structure except for an error of $\overline{\delta}$ we can formulate another MILP to solve the k-MOSS problem (i.e. identify the maximum number of objectives that can be removed for a given maximum allowable approximation error) by replacing constraint 6 by constraint 11:

$$(k\text{-MOSS}) \quad \max OB$$
$$\text{s.t. constraints } 4, 5, 7\text{–}11$$

Step 3: Optimization in the reduced domain. The MOO method (i.e., ε-constraint method) is executed next again but this time in the reduced set of objectives F. This enhances the performance of the standalone method, as it decreases the number of infeasible and/or repeated solutions, which leads to Pareto fronts of higher quality for the same CPU time.

We summarize next the main steps of the algorithm:

1. Generate a set of Pareto-optimal solutions for the dimensionality reduction algorithm.
   (1) Optimize each single objective $f_i \in F_0$ separately, find the maximum and minimum values of each objective f_i. Compose the set of extreme solutions: $S^{(ex)} = \{\overline{s_1}, \underline{s_1}, \ldots, \overline{s_i}, \underline{s_i}, \ldots, \overline{s_K}, \underline{s_K}\}$;
   (2) Define the marginal values of the ε-intervals as follows: $\overline{\varepsilon_i} = \overline{f_i}$, $\underline{\varepsilon_i} = \underline{f_i}$
   (3) Divide each interval $[\underline{\varepsilon_i}, \overline{\varepsilon_i}]$ into $L+1$ subintervals of equal length. Define the sets $E_i = \{\varepsilon_{i,1}, \ldots, \varepsilon_{i,L}\}$;
   (4) For all (or some) pairs of objectives, solve the corresponding bi-criteria models for the limits obtained in the previous step using the ε-constraint method. The resulting solutions compose the set $S^{(bi)}$;
   (5) Conjugate the sets $S^{(bi)}$ and $S^{(ex)}$: $S'' = S^{(bi)} \cup S^{(ex)}$;
   (6) Remove the repeated Pareto solutions from S'' and compose the set S' of the unique Pareto solutions ;
   (7) Normalize the elements of S'. The normalized Pareto solutions from S' compose the set $S^{(norm)'}$;
2. For a given upper bound $\overline{\delta}$ (k-MOSS) or a given number of omitted objectives OB (δ-MOSS), apply the MILP for dimensionality reduction to the set $S^{(norm)'}$ as a basis. Define the reduced objective set F. If $F \neq F_0$ proceed to the next step, otherwise increase L (i.e., number of SO_e models) and go to step 1.2;
3. Solve the reduced space MOO problem.
   (1) Execute the ε-constraint method again for the MOO problem with the reduced set of objectives F. The resulting Pareto solutions compose the set $S^{(red)'}$;
   (2) Conjugate $S^{(red)'}$ and S' : $S^{(final)'} = S^{(red)'} \cup S'$;

(3) Remove the repeated solutions from $S^{(final)'}$ and compose the set $S^{(final)}$ of unique Pareto solutions ;

It is important to remark the following points of the algorithm:

- Note that several objectives from the set F_0 can be redundant or non-conflicting. Hence, the optimization of such objectives may lead to identical solutions. In this case, it is not necessary to apply the ε-constraint for the corresponding bi-criteria model. Hence, step 1.2 should only be performed for the conflicting objectives.
- It is not necessary to solve all possible bi-criteria problems in the first step of the algorithm. In fact, it suffices to generate a large enough set of initial points on the basis of which we will run the MILP.
- In steps 1 and 3, different number of ε-iterations can be used, which affects the overall numerical performance of the algorithm.
- In the typical ε-constraint method, the interval $[\underline{\varepsilon_i}, \overline{\varepsilon_i}]$ is subdivided in $L+1$ subintervals of equal length. It is possible, however, to generate ε-values using other techniques, such as by performing a sampling on the intervals that define each ε-parameter.
- The MILP for dimensionality reduction can be applied iteratively, that is, after step 3 is performed it is possible to go back to step 2 and run the MILP with all the Pareto points generated so far (set $S^{(final)}$).

4. Numerical examples

Two problems were solved to illustrate the computational performance of the method proposed. The models were written in GAMS (Rosenthal, 2008) and solved with the MILP solver CPLEX 12 on an HP Compaq DC5850 desktop PC with an AMD Phenom 8600B, 2.29 GHz triple-core processor, and 2.75 GB of RAM.

Particularly, we solved the examples using our approach and the plain ε-constraint method. To assess the quality of the Pareto sets generated, we employ the hypervolume indicator (Fleischer, 2003) (also known as Lebesgue measure or S-metric). This quality indicator measures the area dominated by the Pareto optimal solutions. Figure 4 shows an example on how this metric would be computed for the bi-criteria case. The larger the indicator is, the better quality the Pareto set has.

4.1. *Case study 1: Design and planning of bioethanol SC*

This case study addresses the optimal design and planning of integrated sugar/bioethanol SCs in Argentina. The production and storage facilities can be installed in 24 sub-regions defined according to the administrative division of Argentina.

We consider all possible configurations of the ethanol/sugar SC as well as all technological aspects associated with its performance, such as production and storage technologies, waste disposal, and transportation alternatives for raw materials and products. Five different technologies, two for sugar production and three types of distilleries, are studied. Sugar mills use sugar cane juice to produce both white and raw sugar. One type of sugar mill generates molasses as a byproduct, whereas the other one produces a secondary honey in addition to sugars. Anhydrous ethanol can be produced by fermentation and subsequent dehydration of different process streams: molasses, honey, and sugar cane juice.

Two different types of storage facilities, warehouses for liquid products and warehouses for solid materials, are considered. It is assumed that materials can be transported by three different types of trucks: heavy trucks with open-box bed for sugar cane, medium trucks for sugar, and tank trucks for liquid products. A detailed mathematical formulation for the problem described above can be found in the works by Mele et al. (2011) and Kostin et al. (2012).

The design problem leads to an MILP model in which the economic performance of the SC is measured via the net present value (NPV), whereas the environmental damage is quantified using 5 environmental metrics: Eco-indicator 99 (EI_{99}), damage to human health (DHH), damage to eco-system quality (DEQ), damage to resources (DR), and global warming potential (GWP_{100}). The goal is to determine the set of Pareto optimal SC configurations that maximize the NPV and minimize environmental impacts.

Following our solution procedure, we first generated a set of Pareto solutions S'. For this, we optimized each single scalar objective separately. This provided the set $S^{(ex)}$ of lower and upper limits for each ε-parameter. Each ε-interval was then split into 6 subintervals, which led to 5 single iterations for each bi-criteria model: $|E_i| = 5, \forall i$. Five bi-criteria models "NPV vs. environmental metric" were thus constructed and solved keeping the NPV as main objective function and transferring the environmental indicators to auxiliary ε-constraints. Hence, 25 iterations were performed in total. The resulting 25 Pareto-solutions were conjugated with the extreme solutions from $S^{(ex)}$ composing the set S''. The repeated solutions were then removed from S'', which led to 30 unique Pareto points that formed the set S'.

We next normalized the elements of S'. The NPV values are normalized as follows:

$$f_i^{(norm)}(s_p) = \frac{\overline{f_i} - f_i(s_p)}{\overline{f_i} - \underline{f_i}} \quad \forall s_p \in S'', i = 1 \tag{12}$$

where $\overline{f_i}$ and $\underline{f_i}$ denote the maximum and minimum values of objective f_i, i.e., $\overline{f_i} = f_i(\overline{s_i})$ and $\underline{f_i} = f_i(\underline{s_i})$. In contrast, the normalized values of the environmental indicators (which are minimized) were calculated as follows:

$$f_i^{(norm)}(s_p) = \frac{f_i(s_p) - \underline{f_i}}{\overline{f_i} - \underline{f_i}} \quad \forall s_p \in S'', i \neq 1 \tag{13}$$

The dimensionality reduction method was next applied to the set of Pareto-optimal solutions $S^{(norm)'}$ considering a maximum allowable δ-error of zero ($\overline{\delta}$ equal to 0). The MILP identified the objective subset {NPV, GWP_{100}, DR } as feasible solution of the δ-MOSS problem for an approximation error of zero.

We next performed a comparison between the enhanced ε-constraint algorithm and the plain ε-constraint method. For this, we solved the full-space model and the reduced-space model (that optimize only objectives NPV, GWP_{100}, DR) using the ε-constraint method for different number of sub-intervals (iterations).

Table 1 displays the results obtained. Note that for the reduced space problems, the total CPU is the summation of the CPU time spent in the reduced space problems (i.e. step 3), the single objective models (step 1.1) and the bi-objective problems (step 1.3). The total CPU time and number of ε -iterations of the full space method includes as well the CPU time and number of iterations associated with the single objective problems.

As expected, the full-space method leads to more iterations and consequently larger CPU times. Furthermore, the Pareto sets provided by the full-space models are worse than those generated with our approach in terms of hypervolume indicator over the whole range of CPU times.

We applied again the objective reduction method to the set of Pareto-optimal solutions obtained after performing the three steps of our algorithm (i.e., to the set $S^{(final)}$) in order to examine the possibility of further objective reductions. There is no combination of two objectives (i.e., neither {NPV, GWP_{100}} nor {NPV, DR}), leading to a zero δ-error. Thus, only one iteration of the proposed method was performed without any further reduction of the problem dimensionality.

4.2. Case study 2: Optimal infrastructure for hydrogen production

The second case study addresses the sustainable design and planning of the future (potential) hydrogen SCs in Spain. We consider three production technologies, two types of hydrogen storage, and four transportation modes. We provide next a brief description of this SC. Further details can be found in the works by Guillén-Gosálbez et al. (2010), Sabio et al. (2010), and Sabio et al. (2012).

Hydrogen can be produced via either steam methane reforming (SMR), or coal gasification, or water electrolysis. The proposed model also considers two possible alternatives for physical storage of hydrogen: compressed hydrogen storage and liquefied hydrogen storage. The terrestrial transport of compressed and liquid hydrogen can be carried out using trucks or railroad cars. In addition, pipelines can be constructed to deliver compressed hydrogen. Ships can also be freighted in order to supply maritime regions with hydrogen. These ships can transport hydrogen in both physical forms: either compressed gas or liquid.

The model considers 19 potential locations for the establishment of production and storage technologies that are defined according to the administrative divisions (autonomous communities) of Spain. The aim is to simultaneously minimize the total discounted cost (TDC) of the hydrogen SC and its environmental impact quantified via the following 8 environmental LCA indicators: damage to human health caused by carcinogenic substances (CS), damage to human health caused by respiratory effects (RE), damage to human health caused by climate change (CC), damage to human health caused by ozone layer depletion (OLD), damage to ecosystem quality caused by ecotoxic substances (ES), damage to ecosystem quality caused by acidification and eutrophication (AE), damage to minerals (DM), and damage to fossil fuels (DFF).

Each scalar objective was first optimized separately in order to identify the extreme limits for each single objective and compose the set $S^{(ex)}$. The associated intervals were then split into 6 subintervals ($L = 5$). Eight bi-criteria problems "TDC vs. environmental impact" were constructed and then solved for each limit in E_i, resulting in 40 iterations in total. After conjugating the sets $S^{(bi)}$ and $S^{(ex)}$ and filtering the repeated solutions, 45 unique Pareto solutions were identified.

We normalized next the solutions according to Eq. 13 and applied the dimensionality reduction technique to the resulting set. For $\overline{\delta} = 0.015$, the reduced objective subset $F = \{TDC, RE, DFF\}$ was found. We solved next the full-space and reduced-space model for different number of ε-iterations. Table 2 shows the computational performance of the full-space and reduced-space models. The CPU time and the number of ε-iterations were computed in the same manner as in the first case study. As seen, the enhanced ε-constraint method outperforms the traditional one in terms of CPU time required and quality of the Pareto sets.

As occurred before, it is not possible to reduce the dimensionality of the problem any further, as there is not any pair of objectives with a δ-error below the threshold.

5. Conclusions

In this paper we have presented a novel method for solving MOO problems with a large number of objectives that integrates a rigorous MILP-based dimensionality reduction method with the classical ε-constraint algorithm. The capabilities of the proposed strategy have been illustrated through its application to the sustainable design of two types of supply chains related with energy applications (i.e., biofuels and hydrogen). It has been clearly demonstrated that the combined use of our rigorous dimensionality reduction method and the traditional ε-constraint method leads to significant savings in time, producing Pareto sets of higher quality in a fraction of the CPU time spent by the stand alone ε-constraint. Furthermore, our method facilitates also the post optimal analysis of the Pareto solutions and provides valuable insight into the relationships between the LCA metrics of concern for decision-makers.

6. Acknowledgement

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7. Notation

Acronyms

EU ETS	European Union Emission Trading Scheme
GHG	greenhouse gas
GrSCM	green supply chain management
GWP_{100}	global warming potential over a 100-year time horizon
DEQ	damage to eco-system quality
DHH	damage to human health
DR	damage to resources
EI_{99}	Eco-indicator 99
LCA	life cycle assessment
MILP	mixed integer linear programming
MOO	multi-objective optimization
MO(X)	multi-objective model
MOSS	minimum objective subset
PCA	principal component analysis
SC	supply chain
SCM	supply chain management
SMR	steam methane reforming
$SO_e(X)$	single objective model
SOOP	single objective optimization problem
TDC	total discounted cost
X	feasible decision variables space
Z	feasible objective space

Indices

e	ε-iterations
i	objectives
n	inequality constraints
n'	equality constraints
p	Pareto solutions

Sets

E_i	ε-values for objective f_i
F_0	original set of objectives
F	reduced set of objectives
S	set of Pareto solutions
S''	set of Pareto solutions of bi-criteria and single criterion models
S'	set of unique Pareto solutions of bi-criteria and single criterion models
$S^{(bi)}$	set of Pareto solutions of bi-criteria models
$S^{(ex)}$	set of extreme solutions
$S^{(final)'}$	final set of Pareto solutions
$S^{(final)'}$	final set of unique Pareto solutions
$S^{(norm)'}$	set of normalized elements of S'
$S^{(red)'}$	set of Pareto solutions of reduced space model

Parameters

$\overline{\delta}$	upper limit for δ-error
$\overline{f_i}$	maximum value of objective f_i
$\underline{f_i}$	minimum value of objective f_i
$f_i^{(norm)}$	normalized value of objective f_i
J	number of Pareto solutions
K	number of objectives in the original space
L	number of ε-values
N	number of inequality constraints
N'	number of equality constraints
$\underline{s_i}$	solution at which objective f_i attains its minimum value
$\overline{s_i}$	solution at which objective f_i attains its maximum value
$YP_{p,p',i}$	binary parameter that takes the value of 1 if solution s_p is better than solution $s_{p'}$ in objective function f_i and 0 otherwise

Variables

$ZD_{p,p'}$	binary variable(1 if solution $s_{p'}$ dominates solution s_p in the reduced Pareto space and 0 otherwise
ZO_i	binary variable (1 if objective f_i is removed from F_0 and 0 otherwise)
$ZOD_{i,p,p'}$	auxiliary binary variable
$\delta_{p,p',i}$	difference between the value of objective f_i in solutions s_p and $s_{p'}$

List of Tables

Table 1. Comparison of the enhanced and plain ε-methods for the first case study

	full-space models			reduced space models					
Number of ε-iterations per objective	3	5	7	3	5	6	7	10	20
Total CPU time, s	1,076	11,417	58,711	233	281	312	363	517	1,463
Total number of ε-iterations	255	3,137	16,819	46	61	94	122	206	534
Number of feasible iterations	76	897	4,947	29	39	46	55	87	280
Unique solutions	11	27	40	26	28	29	31	36	59
Hypervolume	0.0307	0.0877	0.1138	0.0945	0.0857	0.1054	0.1115	0.1232	0.1433

Table 2. Comparison of the enhanced and plain ε-methods for the second case study

	full-space models		reduced space models			
Number of ε-iterations per objective	1	2	3	5	7	10
Total CPU time, s	14,753	104,191	53,718	61,236	79,772	96,214
Total number of ε-iterations	19	274	67	83	107	158
Number of feasible iterations	10	165	53	65	84	118
Unique solutions	7	140	50	62	80	114
Hypervolume	0.0103	0.0252	0.0679	0.0776	0.1077	0.1056

List of Figures

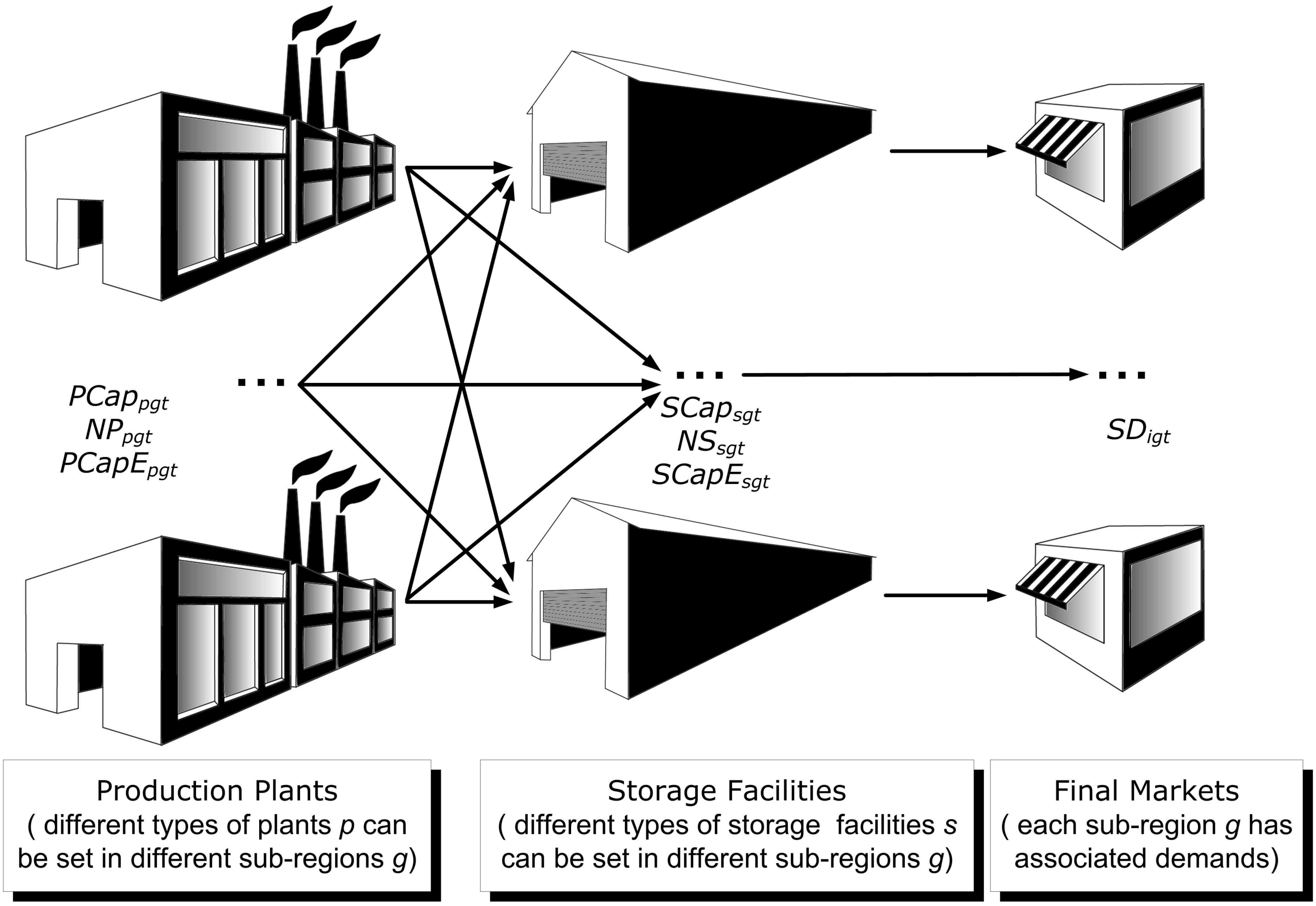


Figure 1. A three-echelon SC

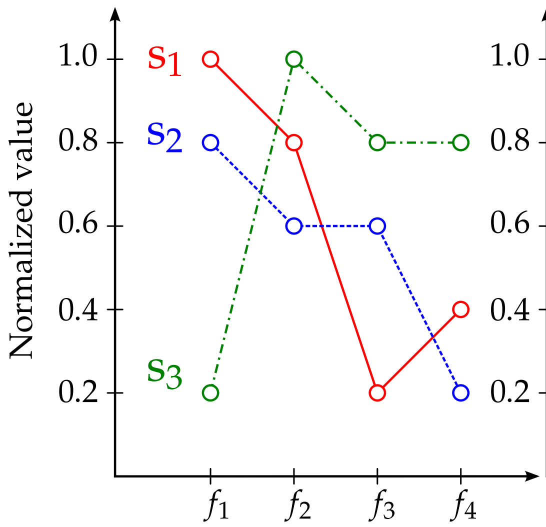


Figure 2a. Dominance structure of the original problem

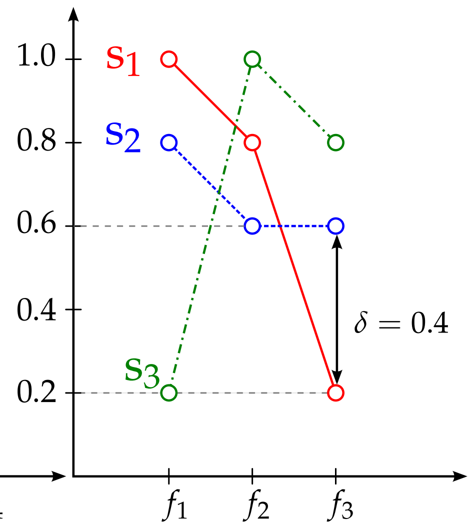


Figure 2b. Dominance structure after removing f_4

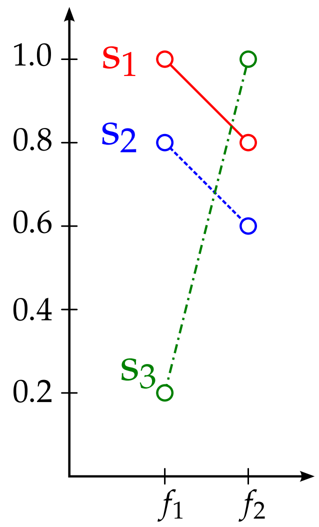
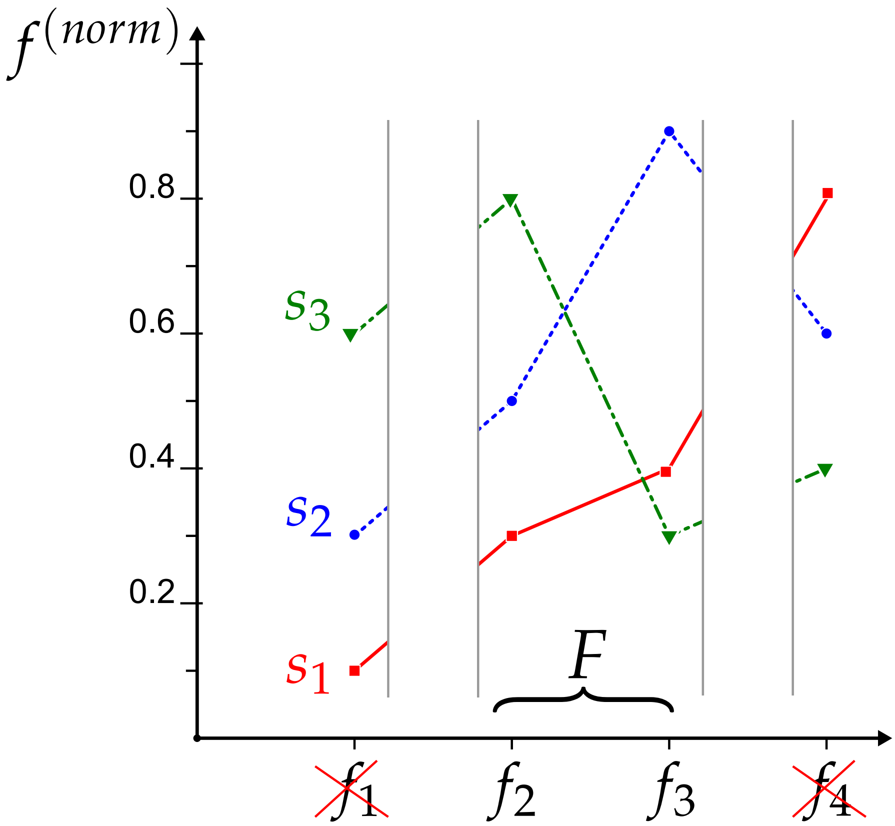


Figure 2c. Dominance structure of the reduced set $\{f_1, f_2\}$



$YP_{p,p',i}$

p,p' \ i	f_1	f_2	f_3	f_4	$ZD_{p,p'}$
1,2	1	1	1	0	0
2,1	0	0	0	1	1
1,3	1	1	0	0	0
3,1	0	0	1	1	0
2,3	1	1	0	0	0
3,2	0	0	1	1	0
ZO_i	1	0	0	1	

Figure 3. Example of the notation used

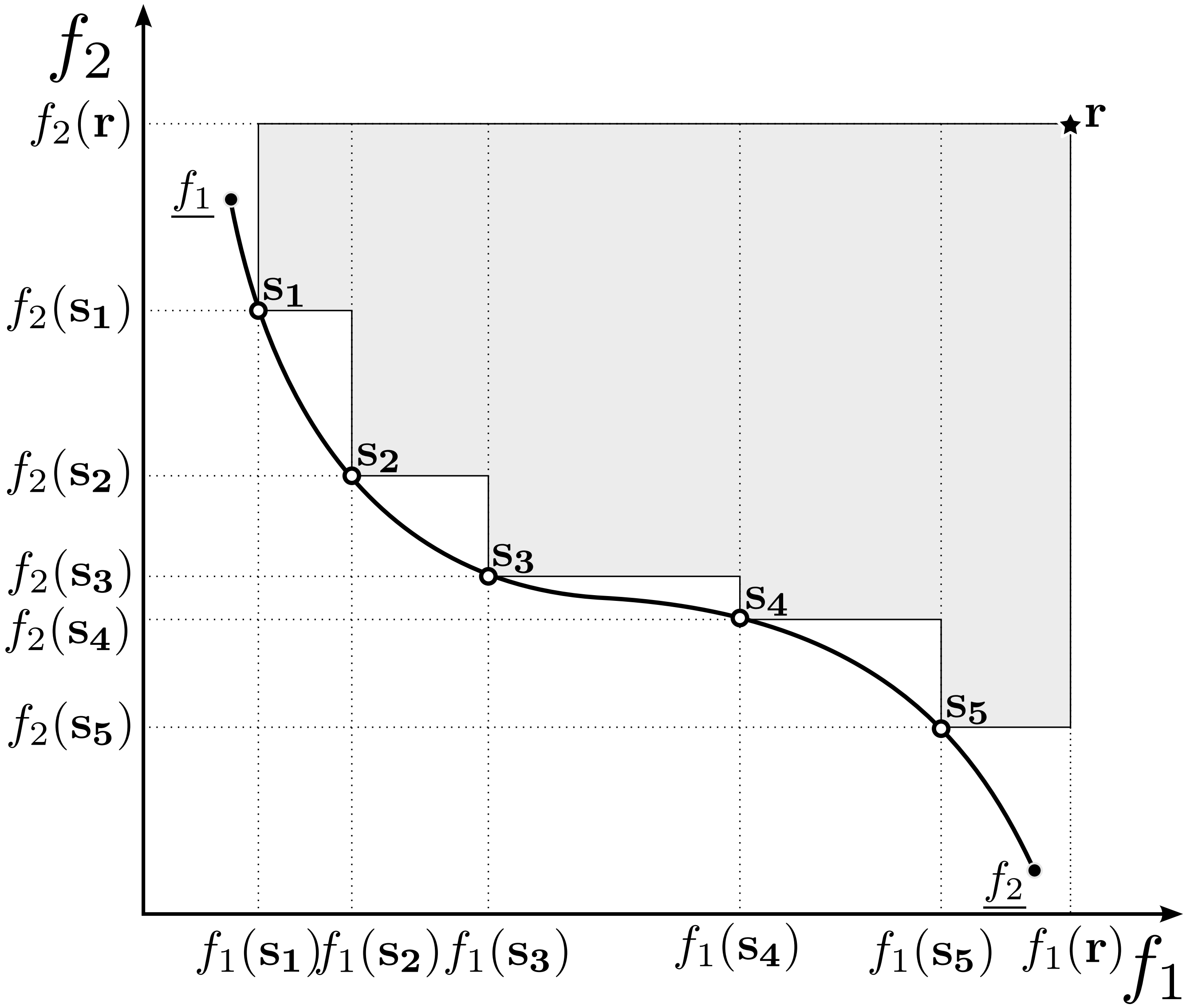


Figure 4. Computation of the hypervolume indicator for a set of Pareto solutions $\mathcal{S} = \{s_1, \ldots, s_5\}$ and the reference point r in a bi-criteria case

Appendices

Four articles were published; one article is currently under review.

A LIST OF PUBLICATIONS

1. **Kostin A.**, Guillén-Gosálbez G., Mele F., Bagajewicz M., Jiménez L. **A novel rolling horizon strategy for the strategic planning of supply chains. Application to the sugar cane industry of Argentina**. *Computers & Chemical Engineering* 35(11), 2540–2563, 2011

2. Mele F., **Kostin A.**, Guillén-Gosálbez G., Jiménez L. **Multi-objective model for more sustainable fuel supply chains. A case study of the sugarcane industry in Argentina**. *Industrial & Engineering Chemistry Research* 50(9), 4939-4958, 2011

3. **Kostin A.**, Guillén-Gosálbez G., Mele F., Bagajewicz M., Jiménez L. **Design and planning of infrastructures for bioethanol and sugar production under demand uncertainty**. *Chemical Engineering Research & Design*, 90(3), 359–376, 2011

4. **Kostin A.**, Guillén-Gosálbez G., Mele F., Jiménez L. **Identifying key life cycle assessment metrics in the multi-objective design of bioethanol supply chains using a rigorous mixed integer linear problem approach**. *Industrial & Engineering Chemistry Research*, 51(14) , 5282–5291, 2012

5. **Kostin A.**, Guillén-Gosálbez G., Jiménez L. **Dimensionality reduction applied to the simultaneous optimization of the economic and life cycle environmental performance of supply chains**. *International Journal of Production Economics*, Under review

B CONTRIBUTIONS TO CONGRESSES

1. **Kostin A.**, Mele F., Bagajewicz M., Jiménez L., Guillén-Gosálbez G. **Integrating pricing policies in the strategic planning of supply chains: a case study of the sugar cane industry in Argentina**. *ESCAPE-20 European Symposium on Computer Aided Chemical Engineering*, Italy, Naples, 2010

2. **Kostin A.**, Guillén-Gosálbez G., Mele F., Jiménez L. **Optimal design and planning of integrated bioethanol-sugar supply chains with economic and environmental concerns. A case study of the sugar cane industry in Argentina** . *AIChE 2010 Annual Meeting*, USA, Salt Lake City, 2010

3. **Kostin A.**, Mele F., Guillén-Gosálbez G. **Multi-objective optimization of integrated bioethanol-sugar supply chains considering different LCA metrics simultaneously**. *ESCAPE-21 European Symposium on Computer Aided Chemical Engineering*, Greece, Chalkidiki, 2011

4. **Kostin A.**, Guillén-Gosálbez G., Mele F., Jiménez L. **Sustainable design of bioethanol supply chains using multi-objective optimization**, *12^{th} Mediterranean Congress of Chemical Engineering*, Barcelona, Spain, 2011.

5. Sabio N., **Kostin A.**, Guillén-Gosálbez G., Jiménez L. **Optimal design and planning of sustainable hydrogen supply chains in Spain: multi-objective optimization coupled with life cycle analysis and principal component analysis**, *12^{th} Mediterranean Congress of Chemical Engineering*, Barcelona, Spain, 2011.

6. **Kostin A.**, Guillén-Gosálbez G., Mele F., Jiménez L. **Objective reduction in multi-criteria optimization of integrated bioethanol sugar supply chains**. *ESCAPE-22 European Symposium on Computer Aided Chemical Engineering*, UK, London, 2012

7. **Kostin A.**, Guillén-Gosálbez G., Mele F., Jiménez L. **Multi-objective optimization of integrated sugar-bioethanol supply chain using dimension reduction techniques**, *ANQUE 's International Congress of Chemical Engineering*, Sevilla, Spain, 2012.

8. **Kostin A.**, Copado-Méndez P. Guillén-Gosálbez G., Jiménez L. **Environmentally conscious optimization of chemical supply chains using dimensionality reduction techniques**. *AIChE 2012 Annual Meeting*, USA, Pittsburgh, 2012

C BOOK CHAPTERS

1. **Kostin A.**, Mele F., Bagajewicz M., Guillén-Gosálbez G., Jiménez L. **Integrating pricing policies in the strategic planning of supply chains: a case study of the sugar cane industry in Argentina**. *Computer-Aided Chemical Engineering*, Pergamon-Elsevier Science Ltd, 2010

2. **Kostin A.**, Mele F., Guillén-Gosálbez G. **Multi-objective optimization of integrated bioethanol-sugar supply chains considering different LCA metrics simultaneously**. *Computer-Aided Chemical Engineering*, Pergamon-Elsevier Science Ltd, 2011

3. **Kostin A.**, Guillén-Gosálbez G., Mele F., Jiménez L. **Objective reduction in multi-criteria optimization of integrated bioethanol-sugar supply chains**. *Computer-Aided Chemical Engineering*, Pergamon-Elsevier Science Ltd, 2012