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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

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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 multi-objective 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.

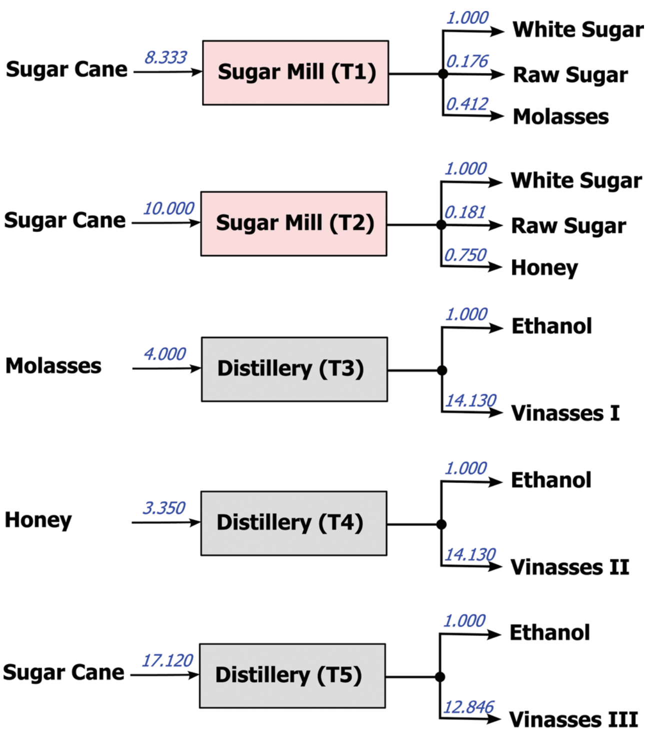

Figure 1. Set of production technologies.

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

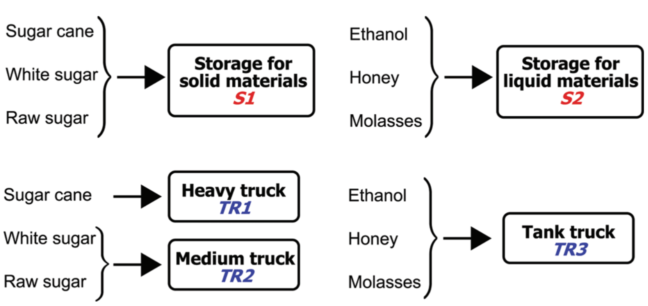

Figure 2. Set of storage and transportation technologies.

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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):

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

subject to

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

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

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:

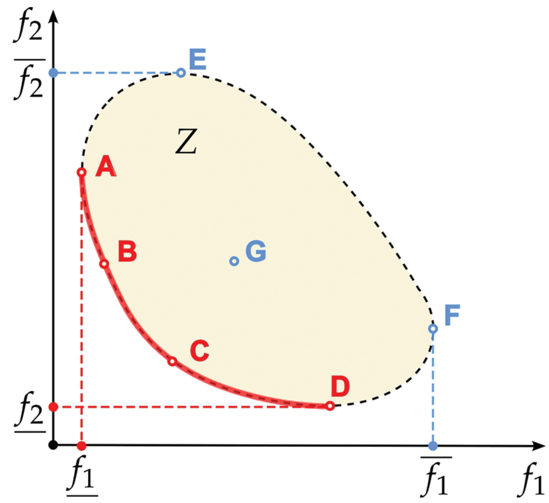

Figure 3. Hypothetical feasible objective space and Pareto optimal front for a MOO problem minimizing both objectives f_1 and f_2. Solutions A, B, C, and D are Pareto-optimal, whereas solutions E, F, and G are nonoptimal. The thin red line denotes the Pareto front.

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:

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

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

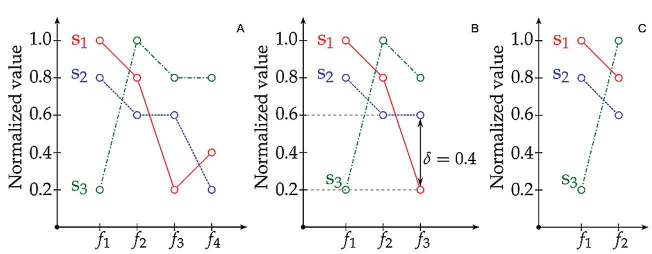

Figure 4. (a) Dominance structure of the original problem. (b) Dominance structure after removing f_4. (c) Dominance structure of the reduced set $\{f_1, f_2\}$.

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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).

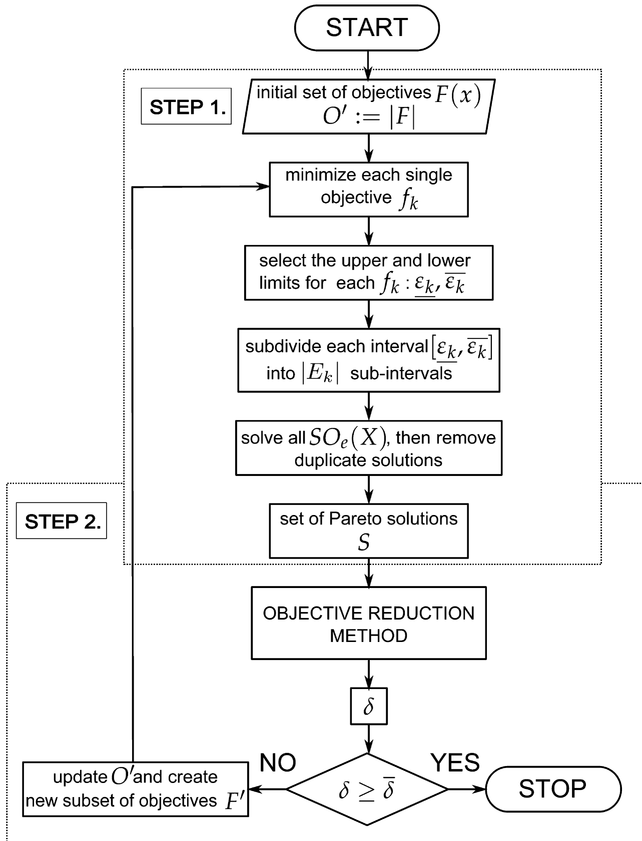

Figure 5. Solution procedure.

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

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

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.

Next, the intervals $[\underline{\varepsilon_k}, \overline{\varepsilon_k}]$ are subdivided into $|E_k|$ subintervals, and model $\mathrm{SO}_\varepsilon(\mathrm{X})$ 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 $\mathrm{YP}_{i,i',k}$ 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 $\mathrm{ZD}_{i,i'}$ 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:

$$\begin{aligned}(L - \sum_k \mathrm{ZO}_k) - L(1 - \mathrm{ZD}_{i,i'}) &\le \sum_k \mathrm{YP}_{i',i,k}(1 - \mathrm{ZO}_k) \\ &\le (L - \sum_k \mathrm{ZO}_k) + L(1 - \mathrm{ZD}_{i,i'}) \quad \forall\, i \ne i'\end{aligned} \tag{6}$$

$$\sum_k \mathrm{YP}_{i',i,k}(1 - \mathrm{ZO}_k) \le (L - \sum_k \mathrm{ZO}_k) - 1 + L\mathrm{ZD}_{i,i'} \quad \forall\, i \ne i' \tag{7}$$

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

$$\delta_{i,i',k} = (f_k(s_{i'}) - f_k(s_i))\mathrm{ZO}_k\mathrm{ZD}_{i,i'} \quad \forall\, i \ne i', k \tag{8}$$

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

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

$$\mathrm{ZOD}_{i,i',k} \le \mathrm{ZO}_k \quad \forall\, i \ne i', k \tag{10}$$

$$\mathrm{ZOD}_{i,i',k} \le \mathrm{ZD}_{i,i'} \quad \forall\, i \ne i', k \tag{11}$$

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

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:

$$\sum_k \mathrm{ZO}_k = \overline{\mathrm{OB}} \tag{13}$$

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

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

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:

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

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

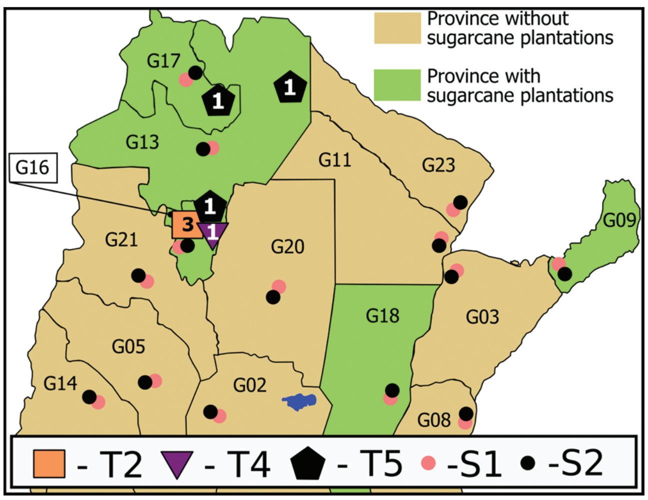

Figure 6. SC configuration for the solution with maximum NPV.

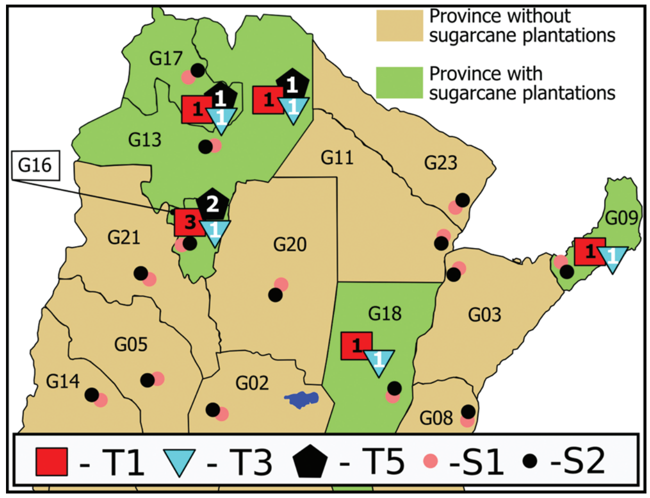

Figure 7. SC configuration for the solution with minimum GWP_{100}.

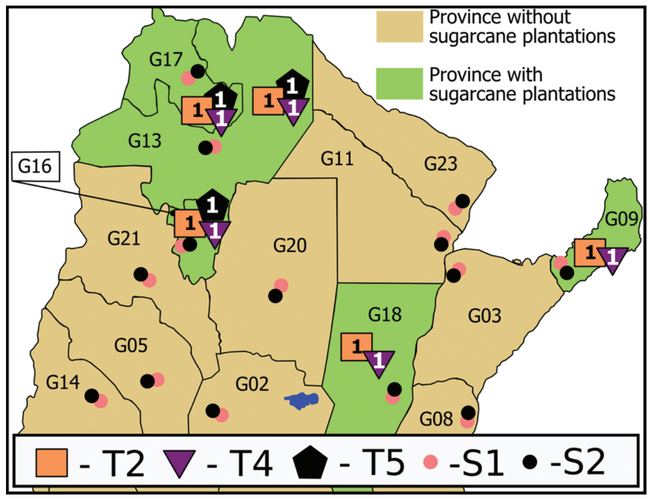

Figure 8. SC configuration for the solution with minimum EI_{99}, DHH, DEQ, and DR.

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 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 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.

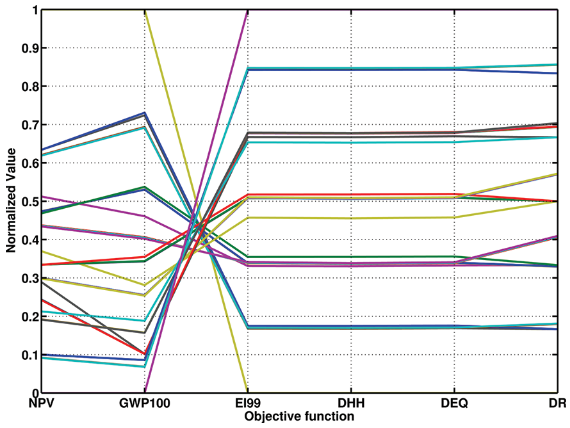

Figure 9. Parallel coordinate plot.

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 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 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.

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

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

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

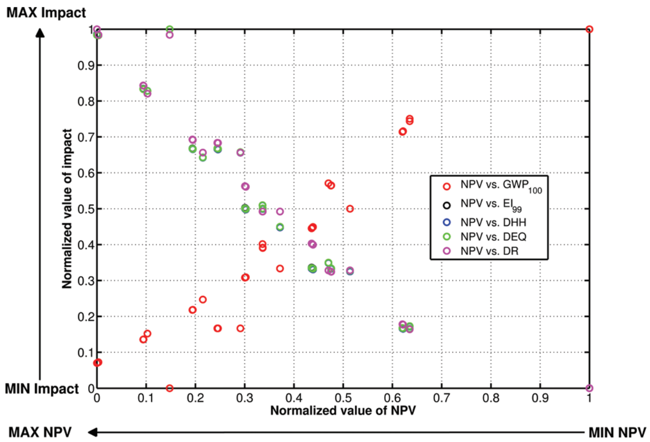

Figure 10. Bicriteria projections of the normalized values of the environmental impacts and NPV.

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

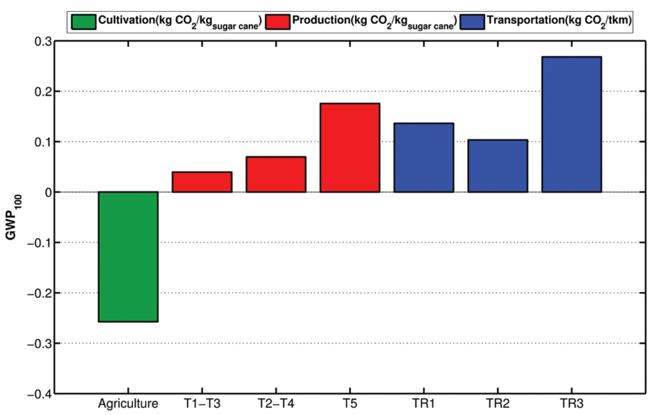

Figure 11. GWP$_{100}$ values for different SC activities. Impact of agriculture is given per kg of sugar cane cultivated. Impact of production is given per kg of sugar cane converted. Impact of transportation is given per ton of material transported 1 km.

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

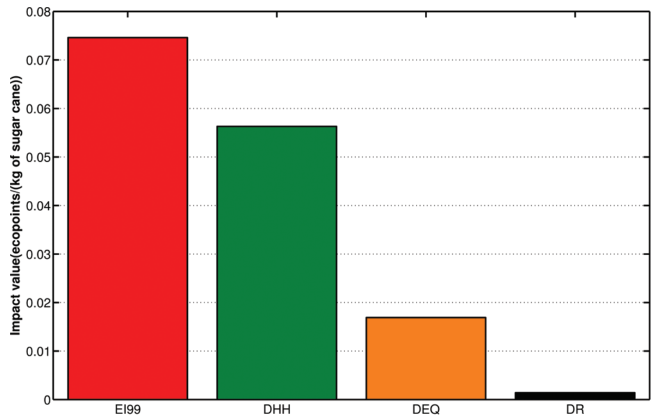

Figure 12. Impact of agriculture in terms of EI$_{99}$, DHH, DEQ, and DR.

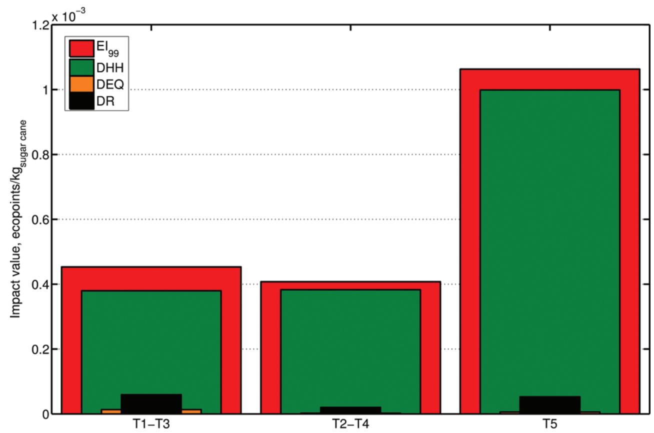

Figure 13. Impact of the different production technologies in terms of EI$_{99}$, DHH, DEQ, and DR. Impact values are given per kg of sugar cane converted.

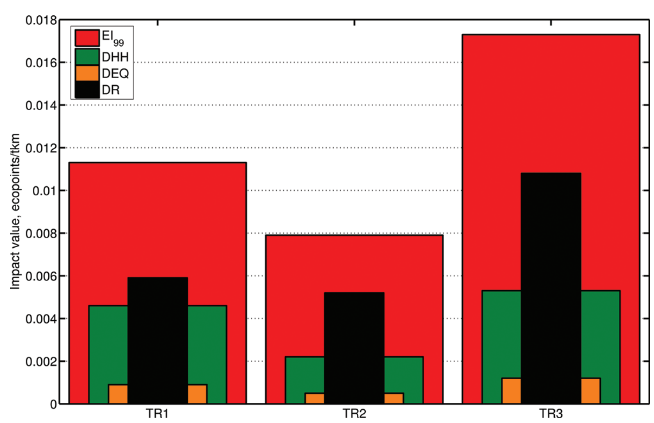

Figure 14. Impact of the different transportation technologies in terms of EI$_{99}$, DHH, DEQ, and DR. Impact values are given per ton of material transported for 1 km.

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.

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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
O' = number of objective functions in subset F'
$\overline{\mathrm{OB}}$ = 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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