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A novel MILP-based objective reduction method for multi-objective optimization: Application to environmental problems

Gonzalo Guillén-Gosálbez

Departament d'Enginyeria Química, Universitat Rovira i Virgili, Av. Països Catalans 26, 43007 Tarragona, Spain

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ABSTRACT

Multi-objective optimization has recently emerged as a useful technique in sustainability analysis, as it can assist in the study of optimal trade-off solutions that balance several criteria. The main limitation of multi-objective optimization is that its computational burden grows in size with the number of objectives. This computational barrier is critical in environmental applications in which decision-makers seek to minimize simultaneously several environmental indicators of concern. With the aim to overcome this limitation, this paper introduces a systematic method for reducing the number of objectives in multi-objective optimization with emphasis on environmental problems. The approach presented relies on a novel mixed-integer linear programming formulation that minimizes the error of omitting objectives. We test the capabilities of this technique through two environmental problems of different nature in which we attempt to minimize a set of life cycle assessment impacts. Numerical examples demonstrate that certain environmental metrics tend to behave in a non-conflicting manner, which makes it possible to reduce the dimension of the problem without losing information.

1. Introduction

Environmental concerns are becoming increasingly important in many scientific areas. The process systems engineering (PSE) community is not an exception to this general trend. A large amount of research is currently being conducted for extending the scope of the analysis carried out in PSE in order to consider environmental aspects. This issue has posed major computational challenges that were discussed in detail in the work by Grossmann and Guillén-Gosálbez (2010). Particularly, one of the main needs in this field is to develop efficient computational tools to assist in the analysis of the trade-off between economic and environmental criteria arising in many engineering problems.

Among the available techniques, multi-objective optimization has emerged as a suitable framework to accomplish this task. This approach allows to incorporate the environmental concerns as additional objectives to be optimized rather than as constraints on the mathematical formulation. Areas of application of multi-objective optimization include the design of chemical plants (Chakraborty & Linninger, 2002; Guillén-Gosálbez, Caballero, & Jiménez, 2008; Stefanis, Livingston, & Pistikopoulos, 1995); the design and scheduling of batch processes (Cavin, Fischer, Glover, & Hungerbühler, 2004; Stefanis, Livingston, & Pistikopoulos, 1997); the selection of solvents in mass separating agent driven technologies (Pistikopoulos & Stefanis, 1998), the design of utility systems (Chang & Hwang, 1996; Papandreou & Shang, 2008); the design of absorption cooling cycles (Gebreslassie, Guillén-Gosálbez, Jiménez, & Boer, 2009, 2010); the design and planning of chemical supply chains (Bojarski, Lainez, Espuna, & Puigjaner, 2009; Guillén-Gosálbez & Grossmann, 2009, 2010; Hugo & Pistikopoulos, 2004; Mele, Espuña, & Puigjaner, 2005; Puigjaner & Guillén-Gosálbez, 2008); and the strategic planning of hydrogen supply chains (Guillén-Gosálbez, Mele, & Grossmann, 2010; Hugo, Rutter, Pistikopoulos, Amorelli, & Zoia, 2005), among others.

Multi-objective optimization provides as output a set of Pareto optimal alternatives that feature the property that it is not possible to find another feasible solution that is better in one of the objectives without necessarily worsening at least one of the others. One of its main advantages is that it allows to articulate the decision-makers' preferences in the post-optimal analysis of the solutions found. This makes it possible to identify solutions that achieve large environmental improvements at a marginal increase in the cost.

The main limitation of multi-objective optimization when applied to environmental problems is that its computational burden grows rapidly in size with the number of environmental objectives. One possible way to overcome this limitation consists of omitting some of them thereby reducing the associated complexity. This has been the prevalent approach followed in the literature. Particularly, from an exhaustive literature review that covered more than 400 citations in the area of multi-objective optimization,

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

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Nomenclature

Indices
- i objective
- s solution

Sets
- I set of objectives
- S set of solutions

Parameters
- $cost_{cw}$ unit cost of cooling water
- Cp_{cw} heat capacity of cooling water
- k total number of objectives
- $OF(s, i)$ value of the i objective of solution s
- $\underline{OF(i)}$ minimum value of objective i
- OB number of objectives omitted
- Q heat exchanged between streams
- M sufficiently large parameter
- t_1 inlet temperature of the cooling water
- T_1 inlet temperature of the hot stream
- T_2 outlet temperature of the hot stream
- $thickness$ thickness of the heat exchanger area
- top total number of operating hours
- U heat transfer coefficient
- $YP(s, s', i)$ binary parameter (1 if solution s is better than solution s' in objective i, i.e., $OF(s, i) \le OF(s', i)$, and 0 otherwise)
- α capital cost parameter
- $\bar{\delta}$ upper bound on the error
- ρ density of steel
- θ_{AP}^{steel} impact caused in acidification per unit of cooling water generated
- θ_{GWP}^{steel} impact caused in global warming potential per unit of cooling water generated
- θ_{TE}^{steel} impact caused in terrestrial ecotoxicity per unit of cooling water generated
- θ_{AP}^{cw} impact caused in acidification per unit of mass of stainless steel produced
- θ_{GWP}^{cw} impact caused in global warming potential per unit of mass of stainless steel produced
- θ_{TE}^{cw} impact caused in terrestrial ecotoxicity per unit of mass of stainless steel produced

Variables
- AP acidification potential
- GWP global warming potential
- $LMTD$ logarithmic mean temperature difference
- m_{cw} cooling water flow rate
- t_2 outlet temperature of the cooling water
- TC total cost
- TE terrestrial ecotoxicity
- $ZD(s, s')$ binary variable (1 if solution s' dominates solution s in the reduced Pareto space and 0 otherwise)
- $ZI(s, s')$ binary variable (1 if s and s' are indistinguishable and 0 otherwise)
- $ZO(i)$ binary variable (1 if objective i is removed and 0 otherwise)
- $ZOD(i, s, s')$ auxiliary binary variable
- $\delta(s, s', i)$ difference between the value of the i objective in solutions s' and s
- $\delta'(s, s', i)$ auxiliary positive variable

Deb and Saxena (2005) concluded that there is an overwhelming majority of them that use only two objective functions. The same happens in the area of environmental engineering, in which the economic performance and a certain environmental metric are typically the objectives optimized (Bojarski et al., 2009; Chakraborty & Linninger, 2002; Guillén-Gosálbez & Grossmann, 2009; Hugo & Pistikopoulos, 2004; Papandreou & Shang, 2008). It should be noted that despite keeping the problem in a manageable size, this approach has the drawback that it requires the decision-makers to articulate their preferences prior to the optimization step.

An alternative approach to reduce the number of objectives is to utilize aggregated environmental indicators defined by attaching weights to the single environmental impacts (e.g., global warming, acidification, ozone layer depletion, etc.). This approach aims at accounting for as many environmental aspects as possible without explicitly including them as single objectives. This requires the definition of weights for every environmental objective and their translation into a single metric. These weights are typically defined by a panel of experts and should ideally represent the views of the society or a group of stake holders. Decision-makers can then incorporate the resulting aggregated indicator into a bi-criteria optimization problem (i.e., cost vs environmental impact) and produce two-dimensional Pareto sets that are easier to calculate and analyze. To this end, researchers in the area have devised different aggregated environmental metrics. Mallick, Cabezas, Bare, and Sikdar (1996) proposed an impact index to measure the potential environmental effects of process wastes. Elliott, Sowerby and Crittenden (1996) presented an indicator calculated using a global mass balance combined with a scoring system for the impact of each pollutant. Biwer and Heinzle (2004) proposed a number of aggregated indices that can be used to optimize the environmental performance of a process in an integrated manner. In the recent past, aggregated methods based on life cycle assessment (LCA) have gained wider acceptante. The Eco-indicator 95 (Goedkoop, 1995) and Eco-indicator 99 methodologies (PRé-Consultants, 2000) are good examples of this type of LCA-based environmental metrics that incorporate scoring or weighting techniques to aggregate several specific performance measures.

So far, the reduction and aggregation of objectives discussed above have relied on the decision-makers' preferences rather than on a systematic mathematical approach. Nevertheless, it is well known that omitting and aggregating objectives may change the dominance structure of the multi-objective problem (Brockhoff & Zitzler, 2006). Particularly, the drawback of leaving certain environmental criteria out of the analysis is twofold. First, we may discard solutions that are optimal in the original space of objectives, but are dominated by another one in the reduced space. More precisely, we can wrongly assume that a process alternative A dominates another solution B (i.e., A is better than B in every objective) and therefore discard solution B, when in fact B is better than A in an environmental metric that was left out of the analysis. Second, two solutions can be indistinguishable in the reduced set of objectives (i.e., show the same performance in all the objectives), when one of them dominates the other one in the original search space.

Hence, at this point, the question that arises is whether it is strictly necessary to include all the environmental metrics in the optimization problem or we can omit some without losing information. In a seminar paper, Brockhoff and Zitzler (2006) introduced a general definition of conflicts between objective sets. They also formally stated the problem of computing a minimum subset of objectives without losing information (denoted as the δ-MOSS problem) and a minimum objective subset of size k with minimum error (k-EMOSS problem). To address these problems, they presented an approximation algorithm with optimum approximation ratio as well as an exact algorithm. Later on, the authors incorporated this approach into hyper-volume based multi-objective evolutionary algorithms in order to improve their performance (Brockhoff & Zitzler, 2007). Deb and Saxena (2005) proposed also a method for reducing the number of objectives in multi-objective optimization based on principal component analysis (PCA). This technique has the limitation that it does not calculate the error of the approximation. The aforementioned objective reduction methods have been mainly applied to academic problems, including the 0-1-knapsack problem (Brockhoff & Zitzler, 2006). To the best of our knowledge, however, they have never been employed in the context of environmental engineering.

In this paper, we propose a novel systematic method for reducing the number of objectives in multi-objective optimization with emphasis on environmental problems. Particularly, given a problem in which a set of environmental metrics are to be minimized, we aim at (i) computing a subset of objectives of given size k such that the error of neglecting the remaining ones is minimized; and (ii) calculating the smallest possible set of original objectives that preserves the original dominance structure except for an error of δ. Our method relies on a novel mixed-integer linear programming (MILP) formulation that can be solved by standard branch and bound techniques. Compared to other objective reduction strategies proposed to date, the advantages of our approach are (i) that it provides a lower bound on the error of omitting objectives; (ii) it can easily be extended in order to accommodate different measures of error; and (iii) it benefits from the efficient branch and bound methods and software applications for solving MILPs. We apply this method to two different multi-criteria problems in which we attempt to minimize a set of LCA metrics. From numerical examples, we conclude that some environmental metrics tend to behave in a non-conflicting manner, so it is possible to lower the dimension of the problem without loosing information.

The paper is structured as follows. In the next section we review concepts and known results on measures for changes in the dominance structure and minimum objectives subsets. In the section that follows, we formally define the problem addressed in this article. The mathematical formulation derived to solve this problem is presented next. Two computational examples are then introduced to test the capabilities of our approach, and the conclusion of the work are finally drawn in the last section of the paper.

2. Background

In the next subsections, we present definitions and results on measures for changes in the dominance structure and minimum objectives subsets. We follow the work by Brockhoff and Zitzler (2006), in which the reader can find further details on this topic.

2.1. Measure of changes in the dominance structure

We consider the following general multi-objective minimization problem MO(X):

$$\mathrm{MO(X)} = \min_{x}\{f(x) := (f_1(x), \ldots, f_k(x)) : x \in X\} \quad (1)$$

with k objective functions $f_i := X \rightarrow R$, $1 \leq i \leq k$, where the vector function $f := (f_1, \ldots, f_k)$ maps each solution $x \in X$ to an objective vector $f(x) \in R^k$.

One of the objectives f_i of MO(X) will represent the economic performance, while the others will quantify the environmental impact. With regard to the quantification of the environmental performance, it should be noted that so far researchers have not yet reached an agreement regarding the environmental indicator that should be used for this purpose (Linninger, Ali, & Stephanopoulos, 1996). Among the possible environmental metrics, those based on LCA principles have attracted an increasing attention in the last years, mainly because they quantify the impact in a holistic manner considering all the stages in the life cycle of a product. This approach avoids local solutions that shift the environmental burdens from one part of the supply chain to another. Methodologies such as the Eco-indicator 95 (Goedkoop, 1995), Eco-indicator 99 (PRé-Consultants, 2000), ReCiPe (Goedkoop et al., 2009), and IMPACT2002+ (Jolliet et al., 2003) are all based on this general philosophy. These approaches rely on a set of indicators that measure the impact in different categories (e.g., carcinogenic effects, climate change, ecotoxicity, acidification, depletion of natural resources, etc.). Moreover, they typically provide normalization and weighting factors for translating these indicators into single environmental metrics that are easy to apply. A common practice in this field is to perform the environmental study on the basis of a reduced number of the aforementioned indicators, since their visualization for a proper analysis become harder as we increase their number. In this context, a systematic tool for reducing the number of environmental objectives can play a major role in identifying redundant indicators thereby facilitating the decision-making process.

The underlying dominance structure considered in this work (assuming that we aim to minimize all the objectives simultaneously) is given by the weak Pareto dominance relation which is defined as follows: $\preceq_{F'} := \{(x, y) | x, y \in X \wedge \forall f_i \in F' : f_i(x) \leq f_i(y)\}$, where F' is a set of objectives with $F' \subseteq F := \{f_1, \ldots, f_k\}$. The following definitions will be used in our analysis.

Definition 1. x weakly dominates y with respect to the objective set F' ($x \preceq_{F'} y$) if $(x, y) \in \preceq_{F'}$.

Definition 2. $x^* \in X$ is called Pareto optimal if there is no other $x \in X$ that dominates x^* with respect to the set of all objectives.

In this work, we propose a systematic method to reduce the dimension of the Pareto set of MO(X). Given a set of objectives $F := (f_1, \ldots, f_k)$, we aim at determining a subset F' of F ($F' \subseteq F$) with a given cardinality such that the error of removing the objectives not contained in F' is minimum. We illustrate this concept with the following example.

2.2. Illustrative example: objective reduction in environmental problems

Consider the 3 Pareto optimal solutions depicted in Fig. 1 that minimize 4 different objectives: cost (f_1), damage to human health (f_2), damage to ecosystem quality (f_3) and depletion of natural resources (f_4). This figure is a parallel coordinates plot (Purshouse & Fleming, 2003) that depicts in the x axis the set of objectives and in the y axis the normalized value attained by each solution. Each line in the figure represents a different Pareto solution, and all of them intersect in at least one point, as none of them dominates any of the others. In general, it will be convenient to normalize the objectives before performing the objective reduction analysis. Different transformation methods can be used for this purpose. The reader is referred to the work by Marler and Arora (2004) for more details on this topic.

In this example, it is possible to remove one objective (i.e., objective 4) without changing the dominance structure of the problem. In other words, for this particular case, we have that $x \preceq_{\{f_1,f_2,f_3\}} y$ if and only if $x \preceq_{\{f_1,f_2,f_3,f_4\}} y$. Further reductions are not possible without modifying the dominance structure. In particular, if we remove f_3, then we have that $x_2 \preceq_{\{f_1,f_2\}} x_1$ although $x_2 \npreceq_{\{f_1,f_2,f_3,f_4\}} x_1$.

In fact, solution x_2 would dominate x_1 in the original 4-dimensional Pareto space $\{f_1, f_2, f_3, f_4\}$ if it showed the same damage in the ecosystem quality category (f_3) than x_1. The difference between the true value of the ecosystem quality damage of x_2 and that required to dominate x_1 in the original space of objectives can be used as a measure to quantify the change in the dominance structure. For this simple example, this value is 0.5. The afore-

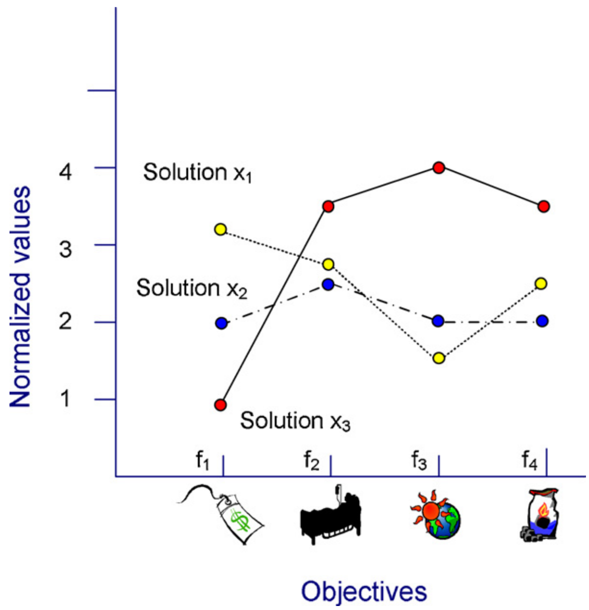

Fig. 1. Illustrative example of dominance structure.

mentioned approach was first suggested by Brockhoff and Zitzler (2006), which proposed computing the error values δ for all solution pairs x, y in order to determine a maximum error of an approximation. Hence, although we can wrongly assume that $x \preceq_{F'} y$, we will always know that x is not worse than y in all objectives by an additive term of δ. As we will show in the next section, the main goal of the analysis conducted in this paper is to calculate subsets of objectives that minimize the δ value.

3. Problem statement

The problem addressed in this article is based on the k-EMOSS problem first introduced by Brockhoff and Zitzler (2006). Given a multi-objective optimization problem that seeks to minimize a set of k objective functions $F := \{f_1, \ldots, f_k\}$, we aim at determining an objective subset $F' \subseteq F$ with a given size j (i.e., $|F'| = j$) such that the dominance structure is preserved with a minimal value of δ. In mathematical terms, we have that for this subset F', the dominance structure of the original set and reduced set of objectives must be the same except for an error equal to δ, that is, the following must hold: $(\preceq_{F'} \subseteq \preceq_F^{\delta}) \wedge (\preceq_F \subseteq \preceq_{F'}^{\delta})$, where the ϵ dominance relation is defined as follows (Zitzler, Thiele, Laumanns, Fonseca, & da Fonseca, 2003): $\preceq_{F'}^{\epsilon} := \{(x, y) | x, y \in X \wedge \forall f_i \in F' : f_i(x) - \epsilon \leq f_i(y)\}$. As we will explain later in the paper, it is possible to utilize our method to solve as well the so called δ-MOSS problem (Brockhoff & Zitzler, 2006), which aims at determining the smallest possible set of original objectives that preserves the original dominance structure except for an error of δ. That is, given a δ value, it is asked to calculate the minimum size of the subset of objectives for which the error of omitting the remaining ones is lower than δ.

4. Proposed methodology

We present next a MILP formulation for solving the problem stated above. We consider a solution subset S ($S \subseteq X$) of a multi-objective problem MO(X) that includes $|S|$ Pareto solutions of dimension k. We introduce the following notation. The parameter $OF(s, i)$ denotes the value of the i objective of solution s. The binary parameter $YP(s, s', i)$ takes the value of 1 if solution s is better than solution s' in objective i (i.e., $OF(s, i) \leq OF(s', i)$) and 0 otherwise. The binary variable $ZO(i)$ is 1 if objective i is removed and 0 otherwise,

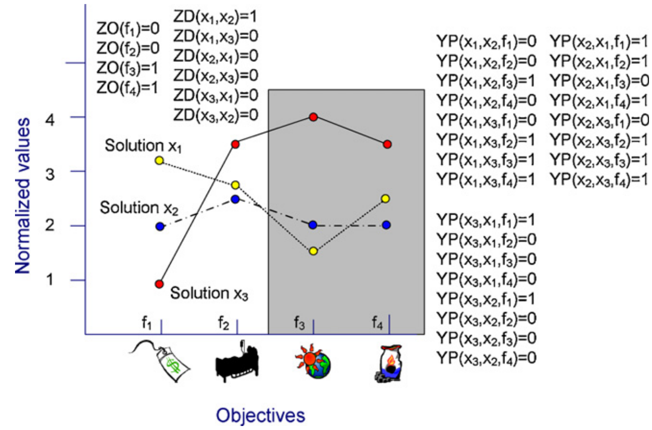

Fig. 2. Notation of the model for the case in which two objectives (f_3 and f_4) are omitted.

and the binary variable $ZD(s, s')$ takes the value of 1 if solution s' dominates solution s in the reduced Pareto space (i.e., the space resulting from removing the objectives i for which $ZO(i) = 1$) and it is 0 otherwise. Fig. 2 shows an example of the application of this notation to the motivating example presented before assuming that we omit objectives f_3 and f_4.

To calculate the binary variable $ZD(s, s')$, we make use of the following constraints:

$$\begin{aligned}(k - \sum_i ZO(i)) - k(1 - ZD(s, s')) &\leq \sum_i YP(s', s, i)(1 - ZO(i)) \\ &\leq (k - \sum_i ZO(i)) + k(1 - ZD(s, s')) \quad \forall s \neq s'\end{aligned} \tag{2}$$

$$\sum_i YP(s', s, i)(1 - ZO(i)) \leq (k - \sum_i ZO(i)) - 1 + kZD(s, s') \quad \forall s \neq s' \tag{3}$$

Recall that solution s' dominates s in the reduced space, if and only if it is better than s in all the objectives that are kept. Consequently, if s' dominates s, then $YP(s, s', i)$ will take the value of 1 for all the objectives for which $ZO(i) = 0$. As a result, the summation of $YP(s, s', i)$ will equal the number of objectives kept in the reduced space. By adding constraint (2) to the model, we ensure that this will only be accomplished if $ZD(s, s')$ is 1. On the other hand, if solution s' does not dominate s, then there will be objectives in which s' will be better than s and others in which the opposite situation will occur. Consequently, the term $\sum_i YP(s, s', i)(1 - ZO(i))$ will be necessarily lower than the cardinality of the set of objectives kept, and constraint (3) will force the binary variable $ZD(s, s')$ to take the value of 0.

Constraint (4) fixes the total number of objectives that are omitted:

$$\sum_i ZO(i) = OB \tag{4}$$

Note that the error of omitting objectives will increase as we impose larger values of OB.

To calculate the error of removing objectives, we make use of the continuous variable $\delta(s, s', i)$, which is the difference between the value of the i objective in solutions s' and s. We define this variable via constraint (5):

$$(OF(s', i) - OF(s, i))ZO(i)ZD(s, s') = \delta(s, s', i) \quad \forall i, s, s' \tag{5}$$

Note that the error $\delta(s, s', i)$ is only calculated for those solutions s dominated by at least another solution s' in the reduced space of objectives, and for those objectives i that are omitted. In contrast, constraint (5) forces the variable $\delta(s, s', i)$ to take a 0 value when s is Pareto optimal in the reduced space and i is a non-omitted objective. Note that in the latter cases, the associated binary variables $ZO(i)$ and $ZD(s, s')$ will take a 0 value, making $\delta(s, s', i)$ equal to 0.

It is possible to linealize the product of the binaries $ZO(i)$ and $ZD(s, s')$ in constraint (5) by making use of the binary variable $ZOD(i, s, s')$ as follows:

$$(OF(s', i) - OF(s, i))ZOD(i, s, s') = \delta(s, s', i) \quad \forall i, s, s' \tag{6}$$

In which $ZOD(i, s, s')$ is defined via the following constraints:

$$ZOD(i, s, s') \le ZO(i) \quad \forall i, s, s' \tag{7}$$

$$ZOD(i, s, s') \le ZD(s, s') \quad \forall i, s, s' \tag{8}$$

$$ZOD(i, s, s') \ge ZO(i) + ZD(s, s') - 1 \quad \forall i, s, s' \tag{9}$$

Constraint (10) is added to prevent the model from accounting for the error $\delta(s, s', i)$ between two solutions s and s' that are non-Pareto optimal in the reduced search space.

$$\begin{aligned} -M\left(\sum_{s''}(ZD(s', s'') - ZI(s', s''))\right) + \delta(s, s', i) \le \delta'(s, s', i) \\ \le M\left(\sum_{s''}(ZD(s', s'') - ZI(s', s''))\right) + \delta(s, s', i) \quad \forall i, s, s' \end{aligned} \tag{10}$$

Here, $\delta'(s, s', i)$ is an auxiliary positive variable that takes the value of $\delta(s, s', i)$ if solution s' is Pareto optimal and dominates solution s, and must lie within some lower and upper bounds otherwise. In this equation, M is a sufficiently large parameter. Moreover, the auxiliary variable $\delta'(s, s', i)$ equals $\delta(s, s', i)$ if all the solutions that dominate s' are indistinguishable (i.e., they dominate each other) in the reduced space of objectives. To take this into account, we introduce the binary variable $ZI(s', s'')$ that has a value of 1 if s' and s'' are indistinguishable in the reduced search space and 0 otherwise. Note that this variable is strictly necessary, as we could otherwise wrongly assume that the error is 0 when in the lower-dimension space all the solutions are indistinguishable. This binary variable is determined via the following constraints:

$$ZI(s, s') \le ZD(s, s') \quad \forall s, s' \tag{11}$$

$$ZI(s, s') \le ZD(s', s) \quad \forall s, s' \tag{12}$$

$$ZI(s, s') \ge ZD(s, s') + ZD(s', s) - 1 \quad \forall s, s' \tag{13}$$

As commented before, the model seeks to minimize the maximum error of omitting objectives. The overall formulation can therefore be expressed as follows:

$$\begin{aligned} (\text{MOR}) \quad & \min \quad \max_{s,s',i} \delta'(s, s', i) \\ & \text{s.t.} \quad \text{constraints } 2 \text{ to } 4,\ 6 \text{ to } 13,\ \text{and } 15 \end{aligned} \tag{14}$$

As mentioned before, we can slightly modify model (MOR) in order to calculate the smallest possible set of original objectives that preserves the original dominance structure except for an error of $\bar{\delta}$. We accomplish this by replacing constraint (4) by Eq. (15), which imposes an upper bound on the maximum allowable error.

$$\delta'(s, s', i) \le \bar{\delta} \tag{15}$$

The modified model (MOR2) can then be expressed as follows:

$$\begin{aligned} (\text{MOR2}) \quad & \max \quad \{\sum_i ZO(i)\} \\ & \text{s.t.} \quad \text{constraints } 2 \text{ to } 3,\ 6 \text{ to } 13,\ \text{and } 15 \end{aligned} \tag{16}$$

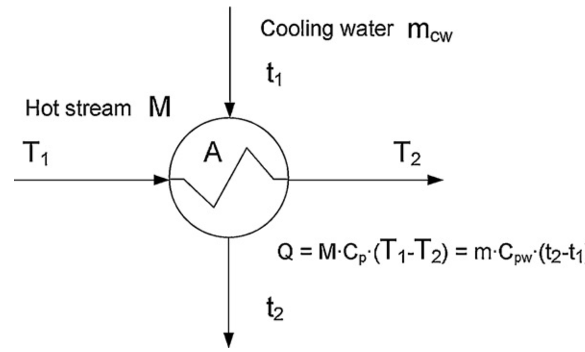

Fig. 3. Case study 1: design of a heat exchanger.

4.1. Remarks

- The Pareto set X of MO(X) might contain an infinite number of Pareto solutions. If this is the case, we shall solve model (MOR) for a reduced number of them, since its computational burden would be prohibitive otherwise. As a result, (MOR) will provide a lower bound on the maximum error of omitting objectives in MO(X). The error provided by (MOR) will also be regarded as a lower bound if the Pareto solutions considered in the analysis are not globally optimal.
- The Pareto solutions should be normalized prior to solving (MOR). This can be done, for instance, by using the following equation:

$$\frac{(OF(s, i) - \underline{OF(i)})}{\underline{OF(i)}} \quad \forall i, s \tag{17}$$

  where $OF(s, i)$ is the original objective function value and $\underline{OF(i)}$ is the minimum value of the objective function i in all the Pareto solutions (i.e., $\underline{OF(i)} = \min_s \{OF(s, i)\} \forall i$). The reader is referred to Marler and Arora (2004) for further details on objective function transformations.
- The proposed method benefits from the efficient branch and bound techniques and software applications that currently exist for solving MILP problems.
- Our algorithm should be used in an iterative manner as follows. We would generate first a set of Pareto solutions in the original search space, and then reduce the number of objectives using (MOR). We would then generate again some Pareto solutions in the reduced search space, and model (MOR) would be re-calculated for these new solutions, providing a new set of objectives to be omitted. This procedure would be repeated until a given termination criterion would be satisfied.

5. Computational results

We tested the capabilities of the proposed method through two case studies: the design of a heat exchanger and the strategic planning of petrochemical supply chains. The examples are described in detail in the following sections.

5.1. Case study 1: multi-objective design of a heat exchanger

This first example serves to illustrate the usefulness of our method in identifying redundant environmental objectives. Particularly, we study the design of a single heat exchanger considering simultaneously economic and environmental criteria (see Fig. 3). Given is a process stream of pure toluene that must be cooled down with water available at 15 °C. The problem consists of determining the set of areas of the heat exchanger that optimize its economic and environmental performance.

The optimization problem seeks to minimize 4 objectives: the total cost and 3 environmental metrics. The problem is formulated as a nonconvex NLP as follows:

$$
\begin{aligned}
\text{(HEX)}\quad & \min \quad (TC, GWP, AP, TE)\\
& \text{s.t.} \quad TC = \alpha \cdot A^{0.65} + cost_{cw} \cdot m_{cw} \cdot top\\
& \quad Q = m_{cw} \cdot Cp_{cw} \cdot (t_2 - t_1)\\
& \quad Q = U \cdot A \cdot LMTD\\
& \quad LMTD = [((T_1 - t_2) - (T_2 - t_1)) \cdot (0.5 \cdot (T_1 - t_2) \cdot (T_2 - t_1))]^{1/3}\\
& \quad GWP = A \cdot thickness \cdot \rho \cdot \theta^{steel}_{GWP} + m_{cw} \cdot top \cdot \theta^{cw}_{GWP}\\
& \quad AP = A \cdot thickness \cdot \rho \cdot \theta^{steel}_{AP} + m_{cw} \cdot top \cdot \theta^{cw}_{AP}\\
& \quad TE = A \cdot thickness \cdot \rho \cdot \theta^{steel}_{TE} + m_{cw} \cdot top \cdot \theta^{cw}_{TE}
\end{aligned}
\tag{18}
$$

The economic performance is measured through the total cost (TC), whereas the environmental performance is quantified via the impact assessment method CML 2001 (Guinée et al., 1992), and more precisely, through the following 3 midpoint categories: global warming potential (GWP), acidification potential (AP), and terrestrial ecotoxicity (TE). The total cost includes the capital and operating cost of the unit. The capital cost is determined from the heat exchanger area, denoted by the continuous variable A, and the parameter α. The value of α was taken from the Guthrie correlations (Douglas, 1998). The operating cost was calculated by multiplying the unit cost of the cooling water (parameter $cost_{cw}$) with the total amount of cooling water consumed during the time horizon, which is given by the flow rate of cooling water (continuous variable m_{cw}) and total number of operating hours (parameter top). The area of the heat exchanger was determined from the amount of heat transferred (parameter Q), the heat transfer coefficient (parameter U); and the logarithmic mean temperature (continuous variable $LMTD$). The LMTD was calculated via the Chen's approximation (Chen, 1991).

The environmental indicators account for the impact caused during the construction and operation of the heat exchanger. It is assumed that the impact during the construction phase is mainly given by the production of the mass of stainless steel contained in the heat exchanger. This impact is available in the environmental database Ecoinvent v2.0 (Althaus et al., 2007). The area of the heat exchanger is translated into the corresponding mass of steel by multiplying the exchange area with the thickness of the tubes (parameter *thickness*) and the density (parameter ρ). The impact per unit of mass of cooling water was also retrieved from Ecoinvent v2.0. Hence, the parameters θ^{steel}_{GWP}, θ^{steel}_{AP}, and θ^{steel}_{TE} represent the impact caused in global warming, acidification and terrestrial ecotoxicity, respectively, per unit of mass of stainless steel produced. On the other hand, the parameters θ^{cw}_{GWP}, θ^{cw}_{AP}, and θ^{cw}_{TE} denote the impact in the same damage categories per unit of cooling water generated. The problem data are displayed in Table 1. A minimum difference of 10 K between the outlet temperature of the cooling water and the inlet temperature of the hot stream was considered.

The underlying trade-off between economic and environmental criteria arising in this problem is as follows. Larger heat exchanger areas lead to lower energy consumption and consequently smaller environmental impacts, as the impact associated with the construction of the equipment unit is small compared to that caused during its operation considering its entire useful life. Hence, the environmental performance can be optimized by increasing the area of the heat exchanger as much as possible. On the other hand, from an economic perspective there is an optimal area that should not be exceeded, since above that point an increase in the capital cost is not compensated by the associated reduction in cooling water expenditures.

We first generated 512 Pareto solutions by applying the ϵ-constraint method, keeping the total cost as main objective and transferring the remaining objectives to auxiliary constraints. To determine the lower and upper limits within which the environmental metrics fall, we optimize each single scalar objective separately. The associated intervals were split into 7 sub-intervals and the model was then solved for the limits of each of them. All the single-objective problems were implemented in GAMS 23.2 and solved with BARON v8.1.5 with an optimality gap of 0%. The solution time for each of these problems ranged between 0.01 and 0.09 CPU s on a computer with an AMD Athlon(tm) II 2.79 GHz processor.

Table 1
Input data of case study 1.

Parameter	Value	Units
$cost_{cw}$	0.2	$\$/m^3$
Cp_{cw}	4.18	kJ/kg K
Q	142.5	kW
t_1	288	K
T_1	365	K
T_2	335	K
Thickness	2	mm
Top	60,000	h
U	0.8	kW/m^2 K
α	2829.25	Cost in $
ρ	8000	kg/m^3
θ^{cw}_{AP}	3.6477×10^{-6}	kg SO2-Eq/kg cooling water
θ^{cw}_{GWP}	8.0120×10^{-4}	kg CO2-Eq/kg cooling water
θ^{cw}_{TE}	7.8820×10^{-7}	kg 1, 4-DCB-Eq/kg cooling water
θ^{steel}_{AP}	2.7067×10^{-2}	kg SO2-Eq/kg steel
θ^{steel}_{GWP}	5.2536	kg CO2-Eq/kg steel
θ^{steel}_{TE}	5.1241×10^{-3}	kg 1, 4-DCB-Eq/kg steel

The solutions were next filtered in order to remove the repeated ones. We obtained finally 14 Pareto optimal solutions that were normalized according to Eq. (17). Table 2 displays the results obtained, whereas Fig. 4 is a parallel coordinates plot that depicts all the solutions in Table 2. Note that all the lines in the figure, each one representing a different Pareto solution, intersect in at least one point, as none of them dominates any of the others. As can be observed, the figure somehow suggests that there is a redundancy in the problem formulation, particularly concerning the 3 environmental metrics. Specifically, the dominance relations $\preceq_{GWP}$, $\preceq_{AP}$ and $\preceq_{TE}$ are all the same.

We applied next model (MOR) to these solutions, minimizing the error of omitting 1 and 2 objectives, respectively. The model featured 6372 constraints, 8444 continuous variables, and 8082 binary variables. The results are summarized in Table 3. As observed, it is possible to discard up to 2 objectives while still keeping the same dominance structure. These results confirmed what we observed

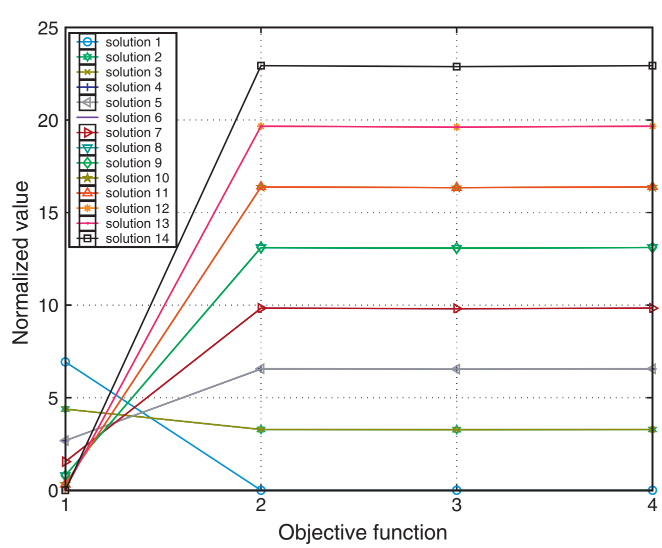

Fig. 4. Parallel coordinates plot of case study 1. The solution numbers refer to those in Table 2. The objectives in the x axis are as follows: (1) total cost, (2) global warming potential, (3) acidification, and (4) terrestrial ecotoxicity.

Table 2
Pareto solutions of case study 1 (“Op.” and “Man.” stand for the operation and manufacturing phases, respectively).

Solution	Area (m^2)	Cost ($)	GWP (kg CO2-Eq)			AP (kg SO2-Eq)			TE (kg 1,4-DCB-Eq)			Time (CPU s)
			Op.	Man.	Total	Op.	Man.	Total	Op.	Man.	Total	
1	7.50	71,088.57	88,036.12	630.45	88,666.57	400.90	3.25	404.15	86.63	0.61	87.24	0.02
2	6.94	69,396.89	90,987.85	583.13	91,570.98	414.34	3.00	417.34	89.53	0.57	90.10	0.05
3	6.94	69,395.48	90,990.90	583.09	91,573.99	414.36	3.00	417.36	89.53	0.57	90.10	0.05
4	6.52	68,268.97	93,927.76	547.73	94,475.49	427.73	2.82	430.55	92.42	0.53	92.95	0.03
5	6.52	68,267.60	93,932.14	547.68	94,479.82	427.75	2.82	430.57	92.43	0.53	92.96	0.05
6	6.19	67,509.59	96,860.13	519.94	97,380.07	441.08	2.68	443.76	95.31	0.51	95.82	0.03
7	6.19	67,508.62	96,864.76	519.90	97,384.66	441.10	2.68	443.78	95.31	0.51	95.82	0.09
8	5.92	67,008.77	99,787.31	497.37	100284.68	454.41	2.56	456.97	98.19	0.49	98.68	0.01
9	5.92	67,008.21	99,791.46	497.34	100288.80	454.43	2.56	456.99	98.19	0.49	98.68	0.06
10	5.69	66,698.58	102710.75	478.59	103189.34	467.73	2.47	470.20	101.07	0.47	101.54	0.06
11	5.69	66,698.34	102713.88	478.57	103192.45	467.74	2.47	470.21	101.07	0.47	101.54	0.02
12	5.50	66,534.19	105631.36	462.66	106094.02	481.03	2.38	483.41	103.94	0.45	104.39	0.05
13	5.50	66,534.13	105633.08	462.65	106095.73	481.03	2.38	483.41	103.94	0.45	104.39	0.03
14	5.34	66,484.51	108549.72	448.94	108998.66	494.32	2.31	496.63	106.81	0.44	107.25	0.08

Table 3
Results of the objective reduction for case study 1.

Problem instance	Total cost	GWP	AP	TE	δ	Time (CPU s)
OB = 1	Kept	Kept	Kept	Omitted	0.00	0.61
OB = 2	Kept	Kept	Omitted	Omitted	0.00	0.97

in Fig. 4, that is, that the three environmental metrics are somehow equivalent. As can be seen in Table 2, the main contribution to the total impact in each case is the consumption of cooling water. Consequently, reducing the cooling water consumption diminishes all the environmental damages simultaneously. This observation explains why the three impacts are somehow equivalent, mainly because they are all highly dependent on the same variable.

5.2. Case study 2: strategic planning of petrochemical supply chains

This second case study was taken from the work by Guillén-Gosálbez and Grossmann (2009), in which the reader can find further details. This is a more complex problem that addresses the optimal design of petrochemical SCs taking into account economic and environmental concerns. It is assumed a superstructure based on a three-echelon SC (production-storage-market) with different available production technologies for plants, potential locations for SC entities and transport links (see Fig. 5). The goal is to determine the SC configuration along with the planning decisions that maximize the NPV and minimize the environmental impact.

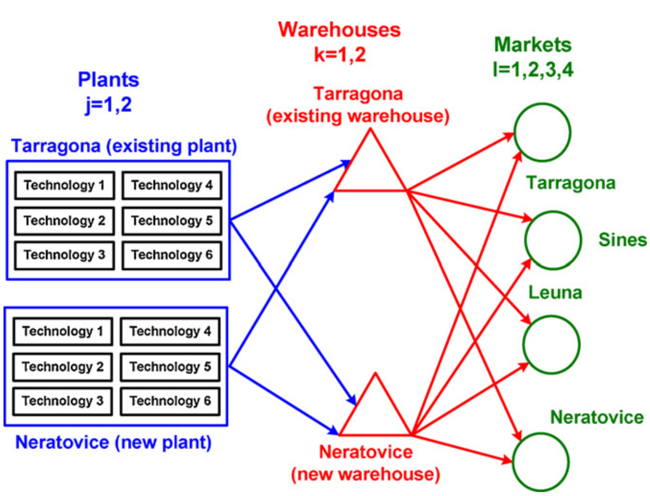

Fig. 5. Case study 2: supply chain superstructure.

We considered 4 environmental impacts that were calculated following the Eco-indicator 99 methodology: damage to human health, damage to ecosystem quality, resources depletion and Eco-indicator 99 points. The Eco-indicator 99 was calculated following the hierarchist perspective combined with the default (average) weighting factors. The goal of the analysis performed in this example was to check if the aggregated Eco-indicator 99 could reproduce the behavior of all the damage categories considered in the formulation.

It should be noted that the original problem introduced in Guillén-Gosálbez and Grossmann (2009) accounted also for the uncertainty of the life cycle inventory of emissions and feedstock requirements associated with the network operation. For the sake of simplicity, uncertainties were not considered in this case. The problem was originally formulated by the authors as a MINLP, in which the nonlinearities were given by a chance constraint used to assess the environmental impact under uncertainty. In this new case, the MINLP was reformulated as a MILP by dropping the aforementioned chance constraint.

We solved the first example in Guillén-Gosálbez and Grossmann (2009) shown in Fig. 5, which led to a multi-objective MILP involving 1968 constraints, 1842 continuous variables and 78 binary variables. We followed a similar procedure as in the previous case, splitting the intervals associated with each objective into 4 subintervals and generating 625 Pareto solutions with the ϵ-constraint method. The points were next filtered prior to solving model (MOR), obtaining 16 Pareto optimal solutions. All the single-objective problems were implemented in GAMS 23.2 and solved with CPLEX 11 with an optimality gap of 0%. The solution time for each of these problems ranged between 0.17 and 0.30 CPU s on the same computer as in the previous example.

Table 4 and Fig. 6 are analogous to Table 2 and Fig. 4. As can be seen, the results suggest again that there is a redundancy in the 3 environmental metrics, although this effect is not as pronounced as in the previous example.

We applied next model (MOR) in order to minimize the error of omitting 1, 2 and 3 objectives, respectively. The model featured 10,082 constraints, 12,163 continuous variables, and 11,444 binary variables. The results are displayed in Table 5. As observed, it is possible to discard up to 2 objectives without changing the dominance structure of the Pareto solutions. Omitting 3 objectives, however, leads to an error of 0.25%. In the latter case, the model determines to keep the Eco-indicator 99 as objective and discard the remaining environmental indicators. In the 2-dimensional search space associated with this problem, the Pareto solution 5 in Table 4, which has a NPV of $\$11.56 \times 10^8$ and 6.01×10^8 Eco-indicator 99 points, dominates the Pareto solution 3, which shows a NPV of $\$11.54 \times 10^8$ and 6.01×10^8 Eco-indicator 99

Table 4
Pareto solutions of case study 2.

Solution	NPV ($)	Human health (DALYs)	Ecosystem quality (PDF m^2 year)	Resources depletion (MJ)	Eco-indicator 99 (points)	Time (CPU s)
1	10.38×10^8	7.00×10^3	4.24×10^8	1.57×10^{10}	5.88×10^8	0.25
2	11.49×10^8	7.16×10^3	4.35×10^8	1.60×10^{10}	6.00×10^8	0.19
3	11.54×10^8	7.16×10^3	4.35×10^8	1.60×10^{10}	6.01×10^8	0.20
4	11.57×10^8	7.17×10^3	4.35×10^8	1.61×10^{10}	6.04×10^8	0.20
5	11.56×10^8	7.18×10^3	4.36×10^8	1.60×10^{10}	6.01×10^8	0.19
6	11.77×10^8	7.22×10^3	4.38×10^8	1.62×10^{10}	6.08×10^8	0.19
7	11.86×10^8	7.33×10^3	4.44×10^8	1.63×10^{10}	6.12×10^8	0.17
8	12.01×10^8	7.32×10^3	4.44×10^8	1.64×10^{10}	6.15×10^8	0.22
9	12.08×10^8	7.34×10^3	4.45×10^8	1.65×10^{10}	6.18×10^8	0.23
10	12.18×10^8	7.45×10^3	4.51×10^8	1.66×10^{10}	6.23×10^8	0.20
11	12.28×10^8	7.45×10^3	4.52×10^8	1.67×10^{10}	6.26×10^8	0.19
12	12.18×10^8	7.49×10^3	4.52×10^8	1.66×10^{10}	6.24×10^8	0.25
13	12.33×10^8	7.54×10^3	4.55×10^8	1.67×10^{10}	6.29×10^8	0.28
14	12.34×10^8	7.57×10^3	4.56×10^8	1.67×10^{10}	6.30×10^8	0.30
15	12.38×10^8	7.67×10^3	4.59×10^8	1.68×10^{10}	6.34×10^8	0.17
16	12.43×10^8	7.90×10^3	4.66×10^8	1.69×10^{10}	6.43×10^8	0.28

Table 5
Results of the objective reduction for case study 2.

Instance	NPV	Human health	Ecosystem	Resources	Eco-indicator 99	δ	Time (CPU s)
Free optimization							
OB = 1	Kept	Omitted	Kept	Kept	Kept	0.00	1.16
OB = 2	Kept	Omitted	Kept	Omitted	Kept	0.00	1.83
OB = 3	Kept	Omitted	Omitted	Omitted	Kept	0.25	2.58
Eco-indicator 99 omitted							
OB = 1		Kept	Kept	Kept	Omitted	0.00	0.97
OB = 2		Kept	Omitted	Kept	Omitted	0.00	1.17
OB = 3		Omitted	Omitted	Kept	Omitted	0.64	2.31

points. In the human health and ecosystem quality categories, however, the dominated solution is slightly better than the former one (7.16×10^3 vs 7.18×10^3 DALYs in human health, and 4.35×10^8 vs 4.36×10^8 PDF m^2 year in ecosystem quality). Particularly, after normalizing these solutions, the maximum error of the approximation is attained in the ecosystem quality category (2.48% with respect to the minimum possible damage in ecosystem quality for solution 3, and 2.73% for solution 5, so $\delta = 2.73–2.48\% = 0.25\%$).

Table 5 shows also the results obtained when the model is forced to omit the Eco-indicator 99 value. As observed, the error is 0 in the first two cases when 1 and 2 objectives are omitted, respectively, and slightly higher than 0.25% (i.e., 0.64%) when 3 objectives are discarded. Particularly, in the latter case (i.e., when 3 objectives are omitted) solution 3 is dominated by solution 5, and solution 10 by solution 12. The maximum error is attained this time in the human health damage category (7.49×10^3 DALYs for solution 12 and 7.45×10^3 DALYs for solution 10).

These results confirmed what we observed in Fig. 6, that is, that the three environmental metrics tend to behave as non-conflicting and that the Eco-indicator 99 is the best metric (i.e., it leads to the minimum error of the approximation) in this particular case study.

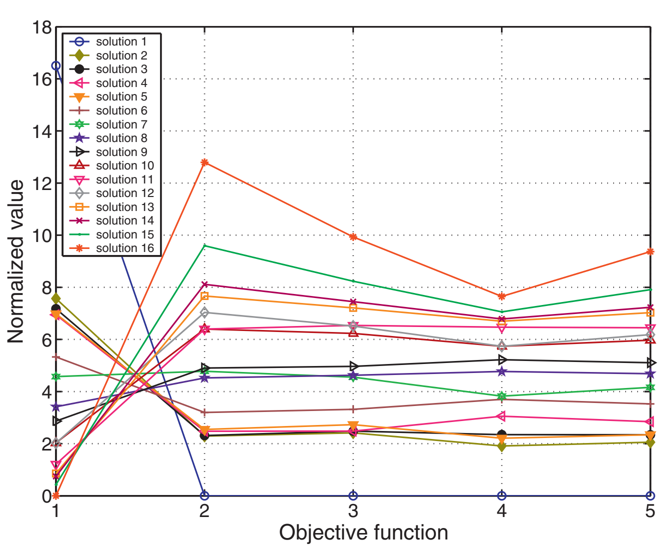

Fig. 6. Parallel coordinates plot of case study 2. The solution numbers refer to those in Table 4. The objectives in the x axis are as follows: (1) NPV, (2) damage to human health, (3) damage to ecosystem quality, (4) resources depletion, and (5) Eco-indicator 99.

6. Conclusions

This work has proposed a novel approach for reducing the number of objectives in multi-objective optimization. The method relies on a novel MILP formulation that seeks to minimize the error of omitting objectives. We have demonstrated the capabilities of this technique through two environmental problems in which several LCA metrics were minimized.

It has been clearly shown that some environmental metrics tend to behave in a non-conflicting manner in certain engineering problems. This observation allows to discard some of them without affecting the Pareto structure of the problem thereby reducing the associated computational burden. The tool presented in this article is intended to enhance the capabilities of multi-objective optimization when applied to environmental problems from the viewpoints of computational efficiency and visualization of the Pareto solutions.

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