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Multiobjective Optimization Using Goal Programming for Industrial Water Network Design

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ABSTRACT: The multiobjective optimization (MOO) of industrial water networks through goal programming is studied using a mixed-integer linear programming (MILP) formulation. First, the efficiency of goal programming for solving MOO problems is demonstrated with an introductive mathematical example and then with industrial water and energy networks design problems, formerly tackled in literature with other MOO methods. The first industrial water network case study is composed of 10 processes, 1 contaminant, and 1 water regeneration unit. The second, a more complex real industrial case study, is made of 12 processes, 1 contaminant, 4 water regeneration units, and the addition of temperature requirements for each process, which implies the introduction of energy networks alongside water networks. For MOO purposes, several antagonist objective functions are considered according to the case, such as total freshwater flow rate, number of connections, and total energy consumption. The MOO methodology proposed is demonstrated to be very reliable as an a priori method, by providing Pareto-optimal compromise solutions in significant less time compared to other traditional methods for MOO.

1. INTRODUCTION

The interactions between industry and environment were practically nonexistent or considered as a secondary concern a few years ago. During the last decades, industrialization has contributed to rapid depletion of natural resources such as water or natural gas. Consequently, there is a real need in industry to ensure minimum natural resources consumption, while maintaining good production levels. In particular, industrial development is always linked to the use of high volumes of freshwater.[1,2] Moreover, a direct consequence of petroleum refineries, as well as chemical and petrochemical industries intensive usage of water, is that wastewater streams contain several contaminants and create an environmental pollution problem.[3]

Twenty percent of the world total water consumption has been recently attributed to industry.[4] However, in a great portion of industrialized countries, this water consumption widely exceeds 50%. By developing cleaner and more economic industrial water networks (IWN), freshwater consumption as well as wastewater can be reduced dramatically. Nevertheless, feasible networks must ensure reasonable costs and do not weaken productivity. In addition, the great majority of involved processes need water with a given quality at a fixed temperature. Hence, huge amounts of energy are also used in order to cool and/or heat water to reach operating temperatures by means of cold and heat utilities. There is thus a critical need in reducing both rejects of contaminants and the consumption of primary resources such as water and energy.

In previous works, IWN allocation problems have been tackled by three main approaches, including graphical (pinch) methodology,[5−8] mathematical programming,[9−12] and synthesis of mass exchange networks.[13−15] The main drawback of the former, although easy to understand, is the difficulty of dealing with several contaminants and complex water networks. On the other hand, due to modern mathematical programming solving algorithms, pinch-based techniques have been competed by mixed-integer programming approaches either linear (MILP) or nonlinear (MINLP). The linear model is generally restricted to simple water networks involving only one contaminant, while the nonlinear one can be applied to more complex networks.[1]

Besides the mathematical model, IWN allocation problems entail several objective functions which are often antagonist between themselves, for example, as discussed above, minimizing resources consumption while maximizing productivity. In fact, very few studies take into account several objectives simultaneously. It is more common to choose a cost objective function to minimize. However, it does not guarantee a simple topology for the network, and it proposes only suitable solutions according to one criteria.

The solution of multiobjective optimization (MOO) problems differs from single objective optimization problems because there is no *global* optimal solution in a mathematical sense, due to the contradictory nature of the set of objectives involved; that is, a solution that minimizes all objectives at the same time does not exist. On the contrary, there is a virtually infinite number of equally significant solutions (i.e., the Pareto front) that are trade-off solutions between the objectives. In fact, the *best* solution (without loss of generality) among the set of solutions should be identified by a decision maker (DM), in accordance with its own criteria.[16,17]

Indeed, the purpose of solving a MOO problem is, in most cases, to find a trade-off solution (or a few of them), and there are several means to achieve this goal. One way is to determine the Pareto front in its totality and choose the trade-off solution a posteriori, or offline. The other set of methods consists in finding one trade-off solution a priori, or online, by solving one or a series of single objective optimization problems. In the former, the advantage is that the totality of the Pareto front is found, with the important drawback that solution times are often prohibitive, since a very big number of sub problems have to be solved, frequently in a stochastic way.[18,19] This drawback is very limiting in the context of large-scale MILP/MINLP (as IWN allocation problems might be), since solution times for a single sub problem is often prohibitive by itself. Moreover, as the number of objective functions increases, so do complexity and solution times. On the other hand, a priori methods do not provide the entire Pareto front, although any solution found is inside it. The essential advantage is that DM preferences are included before the optimization, so the solution of the MOO problem is reduced to the solution of one or a few single objective optimization problems.[16,17] The latter is more than convenient in large-scale optimization problems, for the reasons mentioned above in this paragraph.

Only a few studies have dealt with the MOO of IWN (Vamvakeridou-Lyroudia et al. 2005;[20] Farmani et al. 2006;[21] Mariano-Romero et al. 2007;[22] Tanyimboh et al. 2010[23]). Two studies[20,22] carry out the optimization of single-contaminant distribution networks each one according to two different objectives, such as total freshwater consumption and capital or/and operating costs. While Vamvakeridou-Lyroudia et al.[20] employed fuzzy MOO as the decision-making tool and used stochastic algorithms to find the Pareto front, Mariano-Romero et al.[22] linked the principles of pinch technology with mathematical programming to obtain Pareto-solutions with a heuristic algorithm without using/proposing any decision-making tool. Similarly, Farmani et al.[21] minimized total cost, reliability, and water quality by using a genetic algorithm to construct the Pareto front, and likewise, Tanyimboh et al.[23] by using analytic hierarchy process as the DM.

More recently, Boix et al.[1,2,24] proposed the MOO of industrial water networks both single and multicontaminant by using the ε-constraint method to identify the Pareto front, as well as the simultaneous water-energy network allocation. Among the objective functions, the authors employed, for example, total freshwater consumption, number of connections between processes, and total energy consumed by the network. Also, the authors employed as DM process the TOPSIS[25] (Technique for Order of Preference by Similarity to Ideal Solution) method.

As noted above, none of the previous works have addressed the MOO of IWN by employing a priori solution methods and, what is more, by using goal programming. In fact, all the works are based in the construction of the Pareto front by several means, mostly by stochastic algorithms or mathematical programming along with ε-constraint methodology. However, it is known that these methods encounter some difficulties to deal with large and complex networks and it is always a long task (with high computational times) to build a Pareto front. Furthermore, the problem of water and/or energy network design involve not only continuous variables but also binary variables that make the resolution very difficult in some cases. To overcome these difficulties, we propose here an alternate methodology for solving MOO of IWN in a very efficient way, by using a priori solution methods (specifically goal programming) and specifying DM priorities inside the optimization problem. Case studies include networks tackled before by Boix et al.[2,24] Moreover, we present comparisons among the proposed methodology, other methods, and the results obtained by the other authors, in order to demonstrate its efficiency and reliability to solve MOO problems, generally speaking.

In the subsequent sections, MOO solution methods employed are introduced and explained and every case study is introduced punctually.

2. SOLUTION METHODS FOR MULTIOBJECTIVE OPTIMIZATION

MOO encompasses the solution of optimization problems with two or more objective functions. Generally speaking, a MOO problem is mathematically formulated, as it is illustrated in Problem 1.

$$\min\{f_1(x, y), f_2(x, y), ..., f_{nf}(x, y)\}$$

subject to

$$h(x, y) = 0$$

$$g(x, y) \leq 0$$

$$x \in \mathbb{R}^n, \quad y \in \mathbb{R}^m, \quad h \in \mathbb{R}^p, \quad g \in \mathbb{R}^r \qquad \text{(Problem 1)}$$

As shown above, the problem has *nf* objectives, *n* continuous variables (i.e., x) and m discrete variables (i.e., y) as well as the vectors of equality and inequality constraints (i.e., respectively, $h(x, y)$ and $g(x, y)$).

There are several methods for the solution of MOO problems, where most of them imply the transformation of the original problem in a series of single-objective optimization problems.

2.1. Methods Classification. Solution methods for the solution of MOO problems are generally classified in accordance to the number of solutions generated and the role of the DM inside the problem solution. This classification, adopted by Miettinen[26] and Diwekar[27] is shown in Figure 1.

Methods are initially classified into two groups (Figure 1): generating methods and preference-based methods. The former, as the name indicates, generate one or several Pareto-optimal solutions without taking into consideration DM choices. It is only after all solutions are generated that the DM comes into play. On the other hand, preference-based methods use DM preferences inside the different stages involved in the solution of the problem.

Generating methods are subsequently subdivided into three categories:

- First, the nonpreference methods, as their name indicates, do not consider preference-based solutions.
- Second and third, the a posteriori methods are based on the solution of the original MOO problem by solving a series of single-objective optimization problems in order to find the Pareto front. These two a posteriori methods differ only in the way they are solved, either by scalarization approaches (e.g., ε-constraint or weighting method) or by stochastic algorithms (e.g., simulated annealing or genetic algorithms). Afterward, obtained solutions are evaluated by the DM, which picks the solution to implement. It is important to highlight the significance of the DM in these methods, since the solution method is not capable by itself to provide a unique solution.

Contrariwise, preference-based methods are subdivided into two groups.

- A priori preference methods: DM preferences are initially included into the MOO problem, and then transformed into one or several single-objective problems. Finally, a unique trade-off solution is obtained according to DM preferences included in first place. Reference point method and goal programming are common examples of these methods.

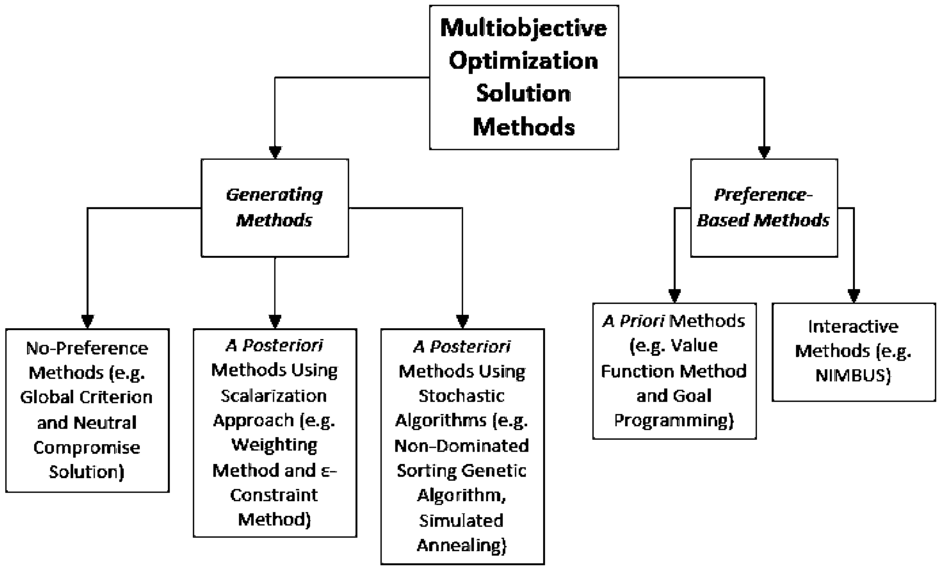

Figure 1. Classification of multiobjective optimization methods.[16]

- Interactive methods: In this group, there is an active interaction of the DM during the resolution process. After each *i*th iteration (i.e., each single-objective problem solution) the DM proposes changes to the Pareto-optimal *i*th values of the objective functions and proposes further changes (either improvement, trade-off, or none) for each one of the objective functions. These preferences are then included into the subsequent iteration. The process stops when the DM is satisfied with the current solution. The most notorious interactive method is the NIMBUS method.[26,28,29]

2.2. A Priori Preference Methods. In the present work, two a priori preference methods, namely, reference point method and goal programming are going to be implemented in an introductive mathematical example to show its usefulness, as well as a posteriori methods coupled with decision-making tools. Afterward, two IWN allocation problems are solved with goal programming whose results are going to be compared against solutions with a posteriori methods found in literature.

2.2.1. Reference Point Methods. These methods are based on the specification by the DM of a reference vector $\overline{z} = [\overline{z}_1,...,\overline{z}_{nf}]$, which includes aspiration levels for each objective function, and then are projected into the Pareto front. In other words, the nearest Pareto-optimal solution to the reference vector is found. This distance can be measured in several ways (cf. Colette and Siarry[17]). Indeed, the distance is measured by an achievement or scalarizing function.[16] Here, the advantage is that the method is able to generate Pareto-optimal solutions no matter how the reference point is specified (i.e., they are attainable or not).[16] The method is illustrated in Figure 2.

There are several achievement functions: in this work, the Tchebychev (or min−max)[17,30] function is implemented (Problem 2).

$$\min\{\max_{i\in F}[w_i(f_i(x) - \overline{z}_i)] + \rho\sum_{i\in F}(f_i(x) - \overline{z}_i)\}$$

subject to

$$h(x) = 0$$

$$g(x) \le 0$$

$$x \in \mathbb{R}^n, \quad h \in \mathbb{R}^p, \quad g \in \mathbb{R}^r \qquad \text{(Problem 2)}$$

In Problem 2, z_i, $\forall i \in F$ are the reference points, $w = [w_1,...,w_{nf}]$ is the weighting vector, $w_i \ge 0$, $\forall i \in F$ and ρ is a positive scalar sufficiently small. Note that the set F is the set containing the objective functions and nf the number of objective functions. One particularity of this method relies on the weighting vector definition, which is defined in turn by vectors z^r and z^v such as $z_i^v > z_i^r$, $\forall i \in F$ according to

$$w_i = \frac{1}{z_i^v - z_i^r}, \quad \forall\, i \in F \qquad (1)$$

The vector z^r is the aspiration vector while z^v is the nadir vector. It is important to note that these vectors can or cannot be attainable; that is, they can or not correspond to feasible alternatives. It is possible to transform Problem 2 in an equivalent minimization problem by adding one additional variable ν and by removing the *max* operator:

$$\min\{\nu + \rho\sum_{i\in F}(f_i(x) - \overline{z}_i)\}$$

subject to

$$\nu \ge w_i(f_i(x) - \overline{z}_i), \quad \forall\, i \in F$$

$$h(x) = 0$$

$$g(x) \le 0$$

$$x \in \mathbb{R}^n, \quad h \in \mathbb{R}^p, \quad g \in \mathbb{R}^r \qquad \text{(Problem 3)}$$

According to Collette and Siarry,[17] for this method to well behave, it is necessary to be capable of choose wisely the reference vector with the purpose of assuring the solution obtained to be consistent with the original problem. Moreover, this method only allows to find Pareto-optimal solutions inside nonconvex regions under certain conditions (see Messac et al.[31]).

2.2.2. Goal Programming. In contrast to reference point method, goal programming does not constraint to work in a convex region. This method consists in transforming the MOO problem in a single-objective problem in the following way:[17] Let $goal = [goal_1,..., goal_{nf}]$ be the vector that contains the levels of aspiration (i.e., the goals) of each objective

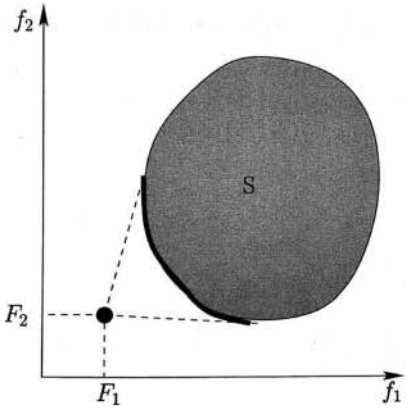

Figure 2. Reference point method.[17]

function, and $d^+ = [d_1^+,..., d_{nf}^+]$, $d^- = [d_1^-,..., d_{nf}^-]$ new variables associated with each objective function that represents the deviations of the objective function value relative to the goals. With these new definitions, the resultant problem is described by Problem 4.

$$\min \sum_{i \in F} w_i \{d_i^+ \vee d_i^- \vee d_i^+ + d_i^-\}$$

subject to

$$f_i(x) + d_i^- - d_i^+ = goal_i, \quad \forall\ i \in F$$

$$d_i^-, d_i^+ \geq 0, \quad \forall\ i \in F$$

$$h(x) = 0$$

$$g(x) \leq 0$$

$$x \in \mathbb{R}^n, \quad h \in \mathbb{R}^p, \quad g \in \mathbb{R}^r \qquad \text{(Problem 4)}$$

Similar to the reference point method, $w_i \geq 0, \forall i \in F, \sum_{i \in F} w_i = 1$ is a necessary condition. Depending on how it is desired to achieve the goal of each function, a different combinations of d_i^+, d_i^- could be minimized, as it is shown in Table 1.

Table 1. Different Combinations of Deviations[17]

case	deviation value	combination of variables to minimize
The *i*th objective function value is allowed to be greater than or equal to the goal *i*.	positive	d_i^+
The *i*th objective function value is allowed to be less than or equal to the goal *i*.	negative	d_i^-
The *i*th objective function value desired has to be equal to the goal *i*.	null	$d_i^+ + d_i^-$

It is important to highlight that in the two first cases the *i*th objective function value is allowed to go further in the opposite direction, when $d_i^+ \vee d_i^- = 0, \forall i \in F$. Goal programming basis is then to be as close as possible to the minimum of each objective function by allowing positive or negative deviations (Figure 3).

On the other hand, it is important to normalize both objective function values and goals:

$$f_i^{norm}(x) = \frac{f_i(x) - f_i^{\min}}{f_i^{\max} - f_i^{\min}} \quad \forall\ i \in F \tag{2}$$

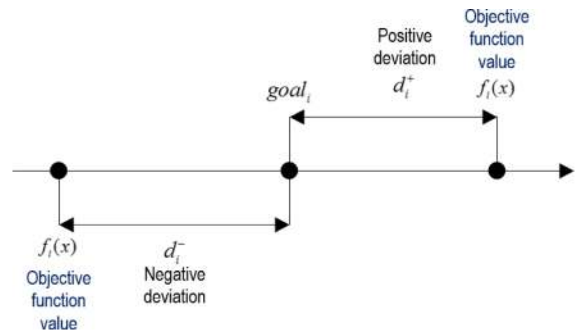

Figure 3. Objective deviations.[32]

$$goal_i^{\text{norm}} = \frac{goal_i - f_i^{\min}}{f_i^{\max} - f_i^{\min}} \quad \forall\ i \in F \tag{3}$$

In eqs 2 and 3, $f_i^{\min}, f_i^{\max}$, $\forall i \in F$ are respectively the minimum and maximum value of each *i*th objective function attained in individual single-objective optimizations.

Finally, it is important to notice that goal programming is the most employed method for multiobjective optimization.[33]

2.3. A Posteriori Preference Methods. These methods are based in the first place on the construction of the Pareto front and then the implementation of multicriteria decision-making (MCDM) tools.

2.3.1. Pareto Front Generation. The Pareto front can be generated traditionally by scalarization approaches or stochastic methods.

Indeed, it can be generated by any method in capacity to produce Pareto-optimal solutions, so even a priori methods are suitable for this task on conjunction with other algorithms.[34] By using these methods, this algorithm deals with changing the weighting coefficients and/or the aspiration levels.

On the other hand, the most common method to generate Pareto-optimal solutions is the ε-constraint method.[26] This method consists in minimizing one of the objective functions at a time and by transforming the others in bounds through inequality constraints. This implies some kind of knowledge of minimum and maximum values of objective functions, and in consequence, the first step is to do single-objective optimizations of each problem separately. The method is stated in Problem 5.

$$\min f_i(x)$$

subject to

$$f_j(x) \leq \varepsilon_j, \quad \forall\ j \in F, \quad j \neq i$$

$$h(x) = 0$$

$$g(x) = 0$$

$$x \in \mathbb{R}^n, \quad h \in \mathbb{R}^p, \quad g \in \mathbb{R}^r \qquad \text{(Problem 5)}$$

In Problem 5, the vector $\varepsilon = [\varepsilon_1,...,\varepsilon_{nf}]$ is the upper bound of the objective functions f_j, $\forall j \in F, j \neq i$. The solution of Problem 5 is always weak Pareto-optimal, and is Pareto-optimal if and only if the solution is unique. Subsequently, to guaranty Pareto-optimality, it is needed to solve *nf* problems.[16] The advantage of this method is that it is in capacity to find every Pareto-optimal solution, even if the problem is nonconvex. Therefore, the Pareto-front obtainment is due to the solution of several single-objective optimizations by changing functions bounds.

Practically, however, it is not always easy to find feasible upper bounds for Problem 5. Also, it can be difficult to determine which problem has to be optimized subsequently. Finally, when the problem has several objective functions, the number of single-objective optimizations that have to be carried out increases substantially, which is not desirable in most cases.

Beyond mathematical programming methods to generate the Pareto-front, stochastic methods have become popular in order to generate the Pareto front in MOO problems. Among these, evolutionary algorithms are the most commonly used since they are easy to implement and are effective. Evolutionary algorithms are based on the emulation of natural selection mechanisms[35] and are particularly appropriated in order to solve MOO problems thanks to their capacity to handle several solutions simultaneously and their ability to tackle different kinds of problems without knowing important information about the problem structure (e.g., derivatives). Nevertheless, evolutionary algorithms require a very significant amount of time to be solved to such an extent that the solution of large-scale problems is prohibitive. The most widely spread evolutionary algorithm is the genetic algorithm and its variants (e.g., NSGA-II[36]).

2.3.2. Decision-Making Tools. A posteriori methods generate several Pareto-optimal solutions, based in the dominance relationship (see Rangaiah and Bonilla-Petriciolet[16] and Collette and Siarry[17]). This relationship allows to filter solutions and to retain only comparable results. Yet, it remains the choice of "the best" solutions according to DM preferences. There are several decision-making tools, but in this study, the interest lies only with TOPSIS based methods.

2.3.2.1. M-TOPSIS. The idea beyond M-TOPSIS is described next.[25] Let $S = [1,...ns]$ be a set with ns alternative solutions of the objective functions and $A_{ns,nf}$ a matrix with ns rows and nf columns:

1. Normalize the decision matrix A, accordingly:

$$A = [a_{i,j}]_{ns,nf} = \frac{f_{i,j}(x)}{\sqrt{\sum_{i\in S} f_{i,j}(x)^2}} \quad \forall\, i \in S, \quad j \in F \tag{4}$$

2. Determine the ideal positive and negative solutions of matrix A:

$$a_{i,j}^{+} = \max_{i}(a_{i,j}) \quad \forall\, j \in F$$
$$a_{i,j}^{-} = \min_{i}(a_{i,j}) \quad \forall\, j \in F \tag{5}$$

3. Compute the distance between each solution and the ideal positive and negative solution using n-dimensional Euclidean distance:

$$D_i^{+} = \sqrt{\sum_{j\in I} w_j (a_{i,j}^{+} - a_{i,j})^2} \quad \forall\, i \in S$$
$$D_i^{-} = \sqrt{\sum_{j\in I} w_j (a_{i,j}^{-} - a_{i,j})^2} \quad \forall\, i \in S \tag{6}$$

4. Calculate the distance of each solution to point O $(\min(D_i^{+}), \max(D_i^{-}))$, $\forall\, i \in S$:

$$R_i = \sqrt{(D_i^{+} - \min_{i\in S}(D_i^{+}))^2 + (D_i^{-} - \max_{i\in S}(D_i^{-}))^2} \quad \forall\, i \in S \tag{7}$$

5. Class solutions in descendant order according to R_i. Consequently, the solution with greater R_i is the best trade-off solution.

2.3.2.2. LMS-TOPSIS. This modification we propose, is based on a linear normalization rather than using the norm as M-TOPSIS does. Indeed, this normalization is the same employed when using goal programming in this study:

$$f_{i,j}^{\mathrm{norm}} = \frac{f_{i,j}(x) - f_j^{\min}}{f_j^{\max} - f_j^{\min}} \quad \forall\, i \in S, \quad j \in F \tag{8}$$

The aforementioned modification is proposed due to poor performance of traditional and M-TOPSIS procedures in nontrivial cases, as it is going to be demonstrated in the subsequent sections.

3. CASE STUDIES

As case studies, we propose an introductory mathematical example to show the followed methodology and two IWA problems, one traditional and one with simultaneous water and energy allocation. For the introductory example, we implemented the two a priori methods addressed above (i.e., reference point method and goal programming) and one a posteriori method, that is, generation of the Pareto front by stochastic methods and decision-making by TOPSIS methods. On the other hand, for the IWA problems, we implemented goal programming in order to compare a priori methods results and the results obtained by Boix et al.[2,24] by implementing a posteriori methods. All a priori implementations were modeled in GAMS.[37] For the MINLP problem (i.e., the introductory example), the outer-approximation solver DICOPT[38] was used coupled with CPLEX[39] and IPOPT.[40,41] For the MILP problems (i.e., the IWA problems), CPLEX[39] was used as the solver. The Pareto front of the introductive example was generated by the genetic algorithm, NSGA-II by using the multipurpose solver MULTIGEN,[42] whose interface is available in Microsoft Excel and ran several times before the construction of the Pareto front. In all cases, weight factors are defined as $w_i = 1/nf$, in order to obtain a trade-off solution without any explicit preference to any objective in particular. In addition, the goal vector in goal programming was defined for all cases as $goal_i = ((f_i^{\max} + 15\, f_i^{\min})/16)$, $\forall i \in F$, and consequently, the normalized goal vector is always $goal_i^{\mathrm{norm}} = 0.062$, $\forall i \in F$ in order to locate goals as close as possible to each function minimum. With the latter in place, the objective in goal programming is then to minimize positive deviation (i.e., d_i^{+}, $\forall i \in F$).

3.1. Introductive Mathematical Example. This biobjective MINLP problem has been proposed by Papalexandri and Dimkou.[43] The formulation is the following:

Table 2. Summary of Results for the Introductive Example

	M-TOPSIS	LMS-TOPSIS	reference point method	goal programming	lower bound	upper bound
f_1	−41.26	−43.84	−43.50	−42.90	−57	−0.92
f_2	41.14	54.54	52.04	48.14	−0.59	329
x_1	0.31	0.13	0.16	0.19	−100	100
x_2	39.98	39.99	40	40	−100	100
x_3	−1.38	−3.86	−3.53	−2.94	−100	100
y_1	0	0	0	0	0	1
y_2	0	0	0	0	0	1
y_3	0	0	0	0	0	1

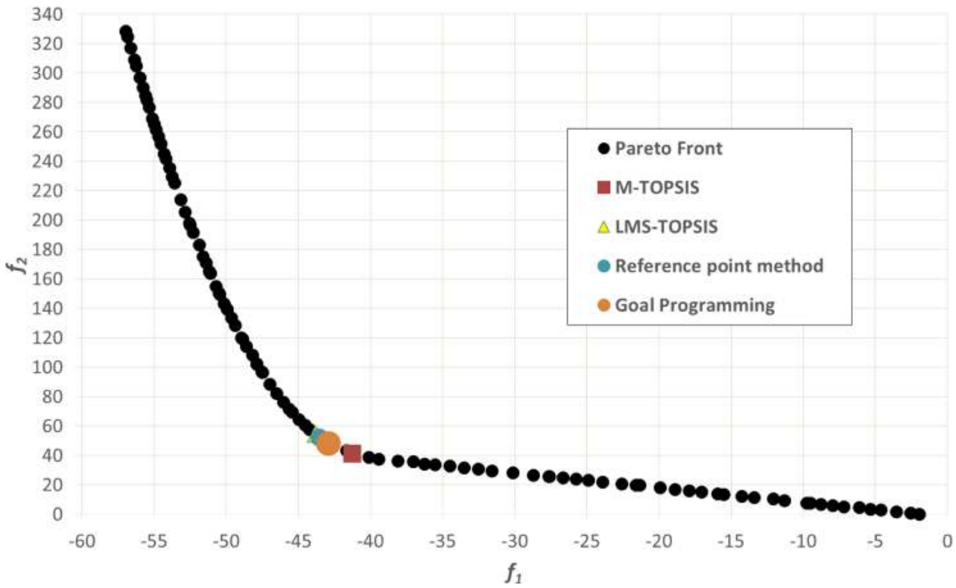

Figure 4. Comparison of obtained solutions with different methods.

$$\min f_1 = x_1^2 - x_2 + x_3 + 3y_1 + 2y_2 + y_3$$
$$\min f_2 = 2x_1^2 + x_3^2 - 3x_1 + x_2 - 2y_1 + y_2 - 2y_3$$
$$s.\ t.$$
$$-3x_1 + x_2 - x_3 - 2y_1 \geq 0$$
$$-4x_1^2 - 2x_1 - x_2 - x_3 + 40 - y_1 - 7y_2 \geq 0$$
$$x_1 + 2x_2 - 3x_3 - 7y_3 \geq 0$$
$$x_1 + 10 - 12y_1 \geq 0$$
$$-x_1 + 10 + 2y_1 \geq 0$$
$$x_2 + 20 - y_2 \geq 0$$
$$-x_2 + 40 + y_2 \geq 0$$
$$x_3 + 17 - y_3 \geq 0$$
$$-x_3 + 25 + y_3 \geq 0$$
$$x_1, x_2, x_3 \in [-100; 100]$$
$$y_1, y_2, y_3 \in [0; 1]$$

3.1.1. Results. The synthesis of results for different methods is illustrated in Table 2 and in Figure 4 over the Pareto front generated with MULTIGEN.

A first analysis of these results leads toward the conclusion that all methods are capable of obtain trade-off solutions. Although, important differences can be noted, possibly due to the normalization method, notably between different TOPSIS implementations. This observations are certainly noted in Tables 3 and 4, which show the normalized gap between a

Table 3. Gap between Solutions Relative to Reference Point Method

variable	percentage error (%) relative to reference point method		
	M-TOPSIS	LMS-TOPSIS	goal programming
f_1	4.0	0.59	1.07
f_2	3.30	0.76	1.18
x_1	0.07	0.02	0.01
x_2	0.01	0.005	0
x_3	1.07	0.16	0.30
mean error	1.69	0.31	0.51

Table 4. Gap between Solutions Relative to Goal Programming

variable	percentage error (%) relative to goal programming		
	M-TOPSIS	LMS-TOPSIS	reference point method
f_1	2.92	1.67	1.07
f_2	2.12	1.94	1.18
x_1	0.06	0.03	0.01
x_2	0.01	0.005	0.0
x_3	0.78	0.50	0.30
mean error	1.18	0.82	0.51

Table 5. Summary of Results with f_1 + 1000

	M-TOPSIS	LMS-TOPSIS	reference point method	goal programming	lower bound	upper bound
f_1	998.52	956.16	977.20	957.10	943.0	999.0
f_2	−0.39	54.54	20.79	48.14	−0.59	329
x_1	0.30	0.13	0.50	0.19	−100	100
x_2	2.28	39.99	23.54	40.0	−100	100
x_3	−0.79	−3.86	−0.50	−2.94	−100	100
y_1	0	0	0	0	0	1
y_2	0	0	0	0	0	1
y_3	1	0	0	0	0	1

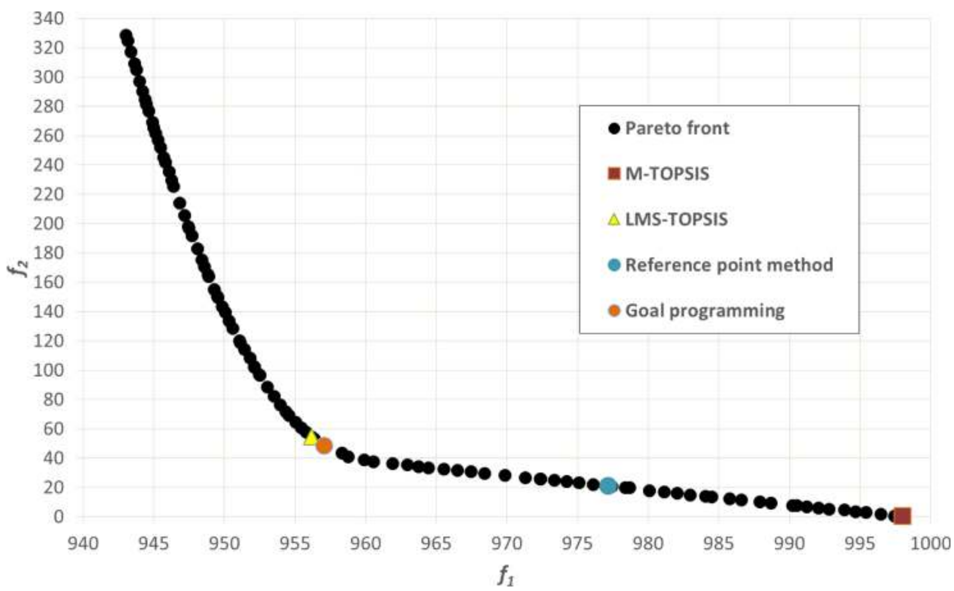

Figure 5. Comparison of results with f_1 + 1000.

priori and a posteriori methods. Moreover, it must be highlighted that binary variables of the problem (i.e., y_1, y_2, y_3) are always equal to zero and also that $x_2 \cong 40$ in all cases. Due to this, the differences between x_1 and x_3 are considerable, since the objective functions are not sufficiently sensitive to these variables.

On the other hand, the problem was exploited in order to analyze the efficiency of the different methods. In fact, f_1 was modified by adding 1000. The objective was to verify if the solutions were the same, since a scalar introduction in an objective function does not change the nature of the optimization problem. Results are shown in Table 5 and Figure 5.

Contrary to the first case, the solution is not the same as it was expected with certain methods. Indeed, M-TOPSIS does not manage to achieve the good solution, while LMS-TOPSIS does achieve it, due to the objective functions normalization proposed. On the other hand, goal programming is able to find the correct solution while the reference point method is not, and is only successful if the aspiration vector is changed. In fact, these results highlight the essential relationship between the reference point method and the aspiration vector. Relative to it, a sensitivity analysis of the solution obtained in function of the chosen vectors was carried out (see Figure 6). It is necessary to clarify that the illustrated variation corresponds to ≈10% of the Pareto front. The latter comports a considerable gap, mainly relative to other methods.

3.2. Industrial Water Network. The formulation of the IWN allocation problem is the same as in previous works.[2,3,9] The way to model a IWN allocation problem is based on the concept of superstructure.[44,45] From a given number of regeneration units and processes, all possible connections between them may exist, except recycling to the same unit. This constraint forbids self-recycles on process and regeneration units, although the latter is often relevant in some chemical processes. For each water-flow rate using process, input water may be freshwater, output water from other process and/or regenerated water. Indeed, output water from a process may be directly discharged, distributed to another process and/or to regeneration units. Similarly, a regeneration unit may receive water from another regeneration unit. For the sake of simplicity and generalization, the problem is built as a set of black boxes.

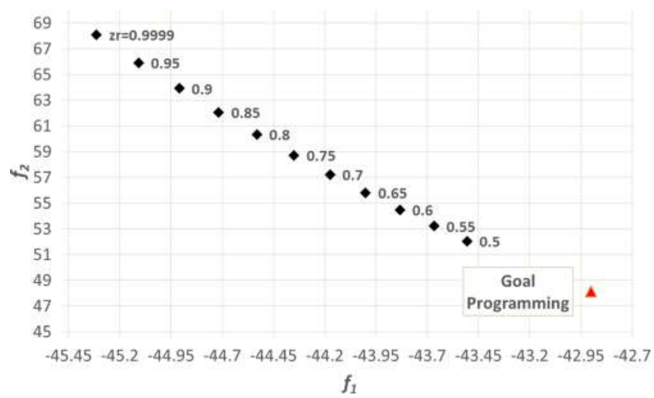

Figure 6. Sensitivity analysis of the results of reference point method in function to the aspiration vector.

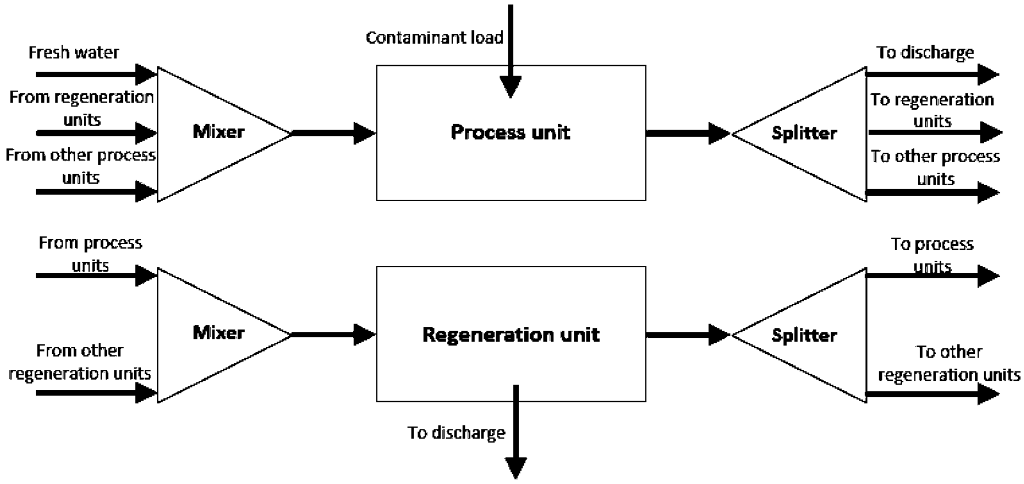

Figure 7. General view of the superstructure for IWN allocation problem.[1]

In this kind of approach, physical or chemical phenomena occurring inside each process is not taken into account. In addition, each process has a contaminant load over the input flow rate of water. A general view of the superstructure is given in Figure 7.

3.2.1. Problem Statement. Given (inputs):

1. The number of processes np. Let $P = \{1,2,...,np\}$ denotes the index set of processes.
2. The number of regeneration units nr. Let $R = \{1,2,...,nr\}$ denotes the index set of regeneration units.
3. The number of components nc. Let $C = \{w,c_1,..., nc\}$ denotes the index set of components (w corresponds to water).
4. The contaminant load for each process (note that water is not a contaminant) M_i^c, $\forall i \in P$, $c \in C$, $c \neq w$.
5. Maximum concentration of a contaminant allowed in the inlet of each process $Cin_{i,c}^{\max}$, $\forall i \in P$, $c \in C$, $c \neq w$.
6. Maximum concentration of a contaminant allowed in the outlet of each process. $Cout_{i,c}^{\max}$, $\forall i \in P$, $c \in C$, $c \neq w$.
7. Output concentration of each contaminant in each regeneration unit. $C_{r,c}^{\text{out}}$, $\forall r \in R$, $c \in C$, $c \neq w$.
8. Minimum and maximum flow rate between any kind of processes and/or regeneration units $minf$ and $maxf$.

Determine (variables):

1. The existence of freshwater input to a process yw_i, $\forall i \in P$.
2. The existence of flow between two processes $yp_{i,j}$, $\forall i, J \in P$, $I \neq J$.
3. The existence of flow between a process and a regeneration unit $ypr_{i,r}$, $\forall i \in P$, $r \in R$.
4. The existence of flow between a regeneration process and a process $yrp_{r,i}$, $\forall r \in R$, $i \in P$.
5. The existence of flow between two regeneration units $yr_{r,s}$, $\forall r,s \in R$.
6. The existence of flow between a process and the discharge yd_i, $\forall i \in P$.
7. The inlet and outlet of each process and regeneration unit for each component Fin_i^c, Fin_r^c, $Fout_i^c$, $Fout_r^c$, $\forall i \in P$, $r \in R$, $c \in C$.

In order to (objectives):

1. Minimize the number of connections.
2. Minimize freshwater consumption.
3. Minimize regenerated water consumption.

3.2.2. Optimization Problem Formulation. The IWN allocation problem comports several objective functions. In this work, number of connections, freshwater consumption, and regenerated water consumption were chosen and are stated in eq 9−11.

$$J_1 = \sum_{i,j \in P, i \neq j} yp_{ij} + \sum_{i \in P} yw_i + \sum_{i \in P, r \in R} (yrp_{r,i} + ypr_{i,R}) \tag{9}$$

$$J_2 = \sum_{i \in P} fw_i \tag{10}$$

$$J_3 = \sum_{r \in R, i \in P} frp_{r,i} \tag{11}$$

The resulting optimization problem to solve is the following:

$$\min(J_1, J_2, J_3)$$

subject to eqs 14−33, 35−40 (described in the Appendix).

3.2.3. Results. The studied network is composed of ten processes and one regeneration unit. The contaminant load of each process is presented in Table 6. The regeneration unit is capable of an outlet concentration of contaminant of 5 ppm, and the value of $minf$ is chosen as 0 T/h. It must be highlighted that the value of these parameters are the same as in Boix et al.[2]

Table 6. Parameters of the Network

process	$Cin_i^{\max}$ (ppm)	$Cout_i^{\max}$ (ppm)	M_i^c (g/h)
1	25	80	2000
2	25	90	2880
3	25	200	4000
4	50	100	3000
5	50	800	30000
6	400	800	5000
7	400	600	2000
8	0	100	1000
9	50	300	20000
10	150	300	6500

Single-objective optimization (i.e., minimizations) were carried out for each objective function, revealing not significantly different lower and upper bound for the latter related to the results of Boix et al.[2] Maximum attained values correspond to the maximum attained among the minimizations of the other objective functions.

objective function	min.	max. attained
no. of connections	10	120
total freshwater flow rate (T/h)	10	255.42
total regenerated water flow rate (T/h)	0	259.51

Subsequently, a multiobjective optimization by using goal programming was accomplished following the same methodology as in the introductive mathematical example. Results are compared with the results of Boix et al.[2] in the Pareto front obtained by the latter authors (Figure 8 and Table 7).

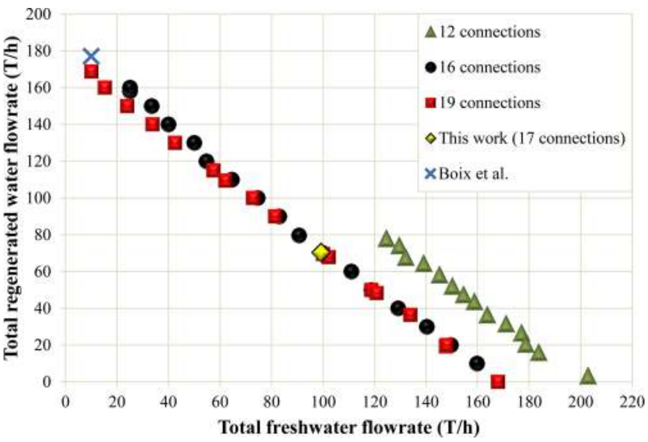

Figure 8. Obtained solution in the Pareto front of Boix et al.[2]

Table 7. Summary of Multiobjective Optimization Results

	this work	Boix et al.[2]
no. of connections	17	17
total freshwater flow rate (T/h)	52.14	10
total regenerated water flow rate (T/h)	120.0	177.24

In Figure 8, the pareto fronts are built with the ε-constraint methodology for each number of connections. Indeed, to deal with MOO, the third objective (number of connections) is fixed as a constraint while the two other objectives are minimized, for more information the reader can referred to Boix et al.[1] As it can be seen from the aforementioned results, the results obtained are indeed different from those of Boix et al.[2] In fact, the former are more suited as a trade-off solution, since all objective functions are in the midst between bounds, while in Boix et al.[2] it can be noted that total freshwater flow rate is at its lower bound, heavily punishing regenerated water consumption. The results obtained are also in accordance to other works, which are also related with the same network (see Bagajewicz and Savelski[9] and Feng et al.[10]).

3.3. Industrial Water and Energy Network. The case of simultaneous water and energy network allocation is tackled in the present section. The problem comports the same elements of an IWN allocation problem, with the addition of energy requirements for each process and/or regeneration units. These energy requirements can be fulfilled by several different means, that is, heat exchangers and/or by warming freshwater in a boiler. In fact, in the current work, we present four different cases by varying the types of utilities and/or energy requirements. The cases are stated as shown in Table 8.

Table 8. Case Description

case	scenario
0	Same case constructed with the same conditions as in Boix et al.[24] Freshwater temperature = 30 °C, only heat exchangers without duty constraints.
1	Freshwater @ 30 °C, heat exchangers with minimum duty = 1000 kW and warm water @ 85 °C.
2	Freshwater temperature @ 30 °C, heat exchangers with minimum duty = 1000 kW and warm water @ 85 and 60 °C.
3	Freshwater @ 10 °C, heat exchangers with minimum duty = 1000 kW and warm water @ 85 and 60 °C.

The last case is added to emulate a situation where the freshwater source is located in a cold area. Indeed, by adding duty constraints to heat exchangers gives the problem an approach closer to reality. Moreover, the case study is based on an existing paper mill facility, as it will be discussed later.

3.3.1. Problem Statement. This type of problem, as said earlier, shares almost all elements with the IWN allocation problem. In fact, all elements in Section 3.2.1 apply, and the following are added or modified:

Given (inputs):

9. The operating temperature of a process Tp_i, $i \in P$.
10. Freshwater temperature Tw, and discharge temperature Td.
11. The operating temperature of a regeneration unit Tr_r, $r \in R$.
12. The maximum inlet flow rate to a process $fmaxp_i$, $i \in P$, and to a regeneration unit $fmaxr_r$, $r \in R$.
13. The minimum and maximum duty of the heat exchanger associated with a process or regeneration unit $minQ$, $maxQ$.

Determine (variables):

8. The existence of a heat exchanger (i.e., cooler or heater) in a process, a regeneration unit or the discharge. $yexp_i^+$, $yexp_i^-$, $yexr_r^+$, $yexr_r^-$, $yexd^+$, $yexd^-$, $i \in P$, $r \in R$

In order to (objectives):

4. Minimize total energy consumption
5. The number of heat exchangers in the network

It is important to note that in the present case study total regenerated water consumption is not considered as an objective function, in order to be in accordance with the case study of Boix et al.[24]

3.3.2. Optimization Problem Formulation. The objective functions related to this case study, according to the aforementioned, are J_1, J_2 and in addition eqs 12 and 13.

Total energy consumption:

$$J_4 = \sum_{i \in P} (Qp_i^+ + Qp_i^-) + \sum_{r \in R} (Qr_i^+ + Qp_i^-) + (Qd^+ + Qd^-) \tag{12}$$

Number of heat exchanges in the network:

$$J_5 = \sum_{i \in P} (yexp_i^+ + yexp_i^-) + \sum_{r \in R} (yexr_i^+ + yexr_i^-) + (yexd^+ + yexd^-) \tag{13}$$

In accordance, the resulting optimization problem is the following:

$$\min(J_1, J_2, J_4, J_5)$$

subject to eqs 14−33, 35−40, 41−46 (described in the Appendix).

3.3.3. Results. The case study is the same as the one treated by Boix et al.,[24] which is in turn an adaptation of a real-world application of a paper mill plant[8] (Figure 9).

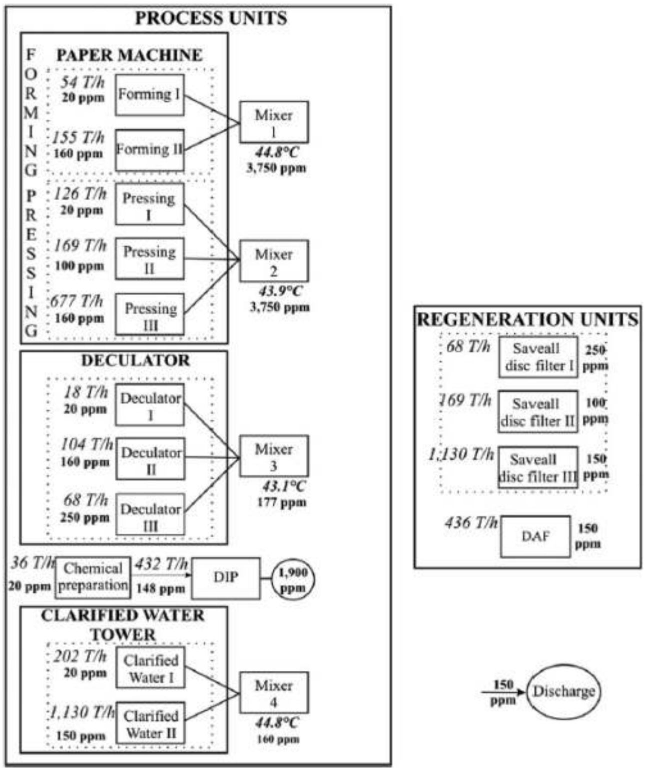

Figure 9. Flowsheet of the paper mill case study.[24]

The case study is made up of 12 processes, and four regeneration units. For this case, *minf* is fixed to 2 T/h, since lower flow rates would imply piping inferior to 1 inch in diameter. These and other parameters value are the same as in Boix et al.[24] Table 9 shows the results of each case. The minimum and maximum attained values correspond to single-objective optimizations.

From Table 9 several items should be pointed out: in the first place, results between the base case and those from Boix et al.[24] make evident significant gaps between the objective functions. Relative to minimum and maximum attained values, results of case 0 are evidently real trade-off solutions. In fact, as goal programming is employed, the latter is assured in comparison to a posteriori methods (i.e., Boix et al.[24] best solution). It is also important to notice that cases offering the option to feed processes with warm water (cases 1, 2, and 3) propose optimal solutions with a low number of heat exchangers (only 4). However, the imposed lower bound for the number of heat exchangers (3) contributes to the design of a more realistic network. Indeed, the presence of heat exchangers could involve higher operating, raw material and energy costs but lower maintenance and capital costs for equipment. Nevertheless, energy consumed by the network in these cases is not highly penalized, and neither the number of connections. In order to provide a deeper analysis on energy, the duty of each exchanger is illustrated in Table 10, as well as cold/warm freshwater flow rate for all cases (Table 11).

Table 10. Heat Exchanger Duties and Location for All Cases

	heat exchanger duty (MW)			
process	case 0	case 1	case 2	case 3
1	1.25			
2				
3	2.91			
4				
5	−1.41	−1.41	−1.41	−1.41
6	0.15			
7				
8				
9				
10	1.64			
11				
12	1.55	2.01	2.01	1.13
R1				
R2	−0.13			
R3	26.27	26.40	26.38	26.08
R4				
discharge	−5.79	−5.90	−5.89	−5.86

From Tables 10 and 11 it is evident that heat exchangers are essential in active regeneration units, since warm freshwater is not allowed to feed the latter. Indeed, the duty of the heat exchanger relative to regeneration unit number 3 is the one that consumer more than 50% of total energy consumption in all cases. On the other hand, processes, regeneration units, or the discharge that have low temperature requirements need necessarily a cooler, as there is not available another source of cooling utility. In the second place, it can be inferred that warm freshwater @ 85 °C lowers significantly the need of exchangers in case 1, and that freshwater @ 60 °C is preferred and sufficient for the other cases. It is to be noted also that in the base case there are exchangers with very low duties, thing that is traduced in very little and less efficient heat exchanger equipment. In addition, it is clear that source freshwater temperature has a very important impact on the network performance. For instance, the total energy consumed in case 3 is significantly higher than in other cases. Moreover, it is important to note that all cases that involve warm freshwater sources comport higher number of connections, since it is evident the preference for the latter than heat exchangers themselves.

Table 9. Summary of Results for the Water and Energy Network

	case 0			case 1			case 2			case 3			Boix et al. (TOPSIS)
objective function	min.	max.	optimal	min.	max.	optimal	min.	max.	optimal	min.	max.	optimal	optimal
no. of connections	20	41	25	26	49	36	26	54	36	26	53	36	35
freshwater consumption (T/h)	377.64	1519.02	452.3	391.55	1519.02	461.35	391.55	1519.02	461.35	388.39	1519.02	458.96	389.3
energy consumption (MW)	34.95	129.28	41.1	36.81	171.68	41.94	36.77	189.82	41.94	42.58	177.37	49.73	36.62
no. of heat exchangers	8	17	9	3	16	4	3	16	4	3	16	4	10

Table 11. Summary of Freshwater Sources Results for All Cases

	freshwater flow rate (T/h)								
	case 0	case 1		case 2			case 3		
process	@ 30 °C	@ 30 °C	@ 85 °C	@ 30 °C	@ 85 °C	@ 60 °C	@ 10 °C	@ 85 °C	@ 60 °C
1	53.71	29.51	17.85	14.63		32.72	11.94		41.78
2	18.65	9.44		9.44			12.18		13.39
3	125.33	61.07	39.90	27.82		73.15	22.86		89.44
4		52.33	11.73	42.56		21.50	2.45		4.03
5									
6	15.97	13.64	2.32	11.71		4.26	7.81		8.16
7									1.93
8	16.30	16.30		16.30			11.0		
9									
10	176.40	150.74	25.66	129.36		47.04	86.75		89.98
11	22.17								35.53
12	23.77	30.86		30.86			12.92		

4. CONCLUSIONS

In this work, it is addressed the IWN allocation problem by multiobjective optimization using a priori methods, more specifically speaking, goal programming. This method has never been explored to the case of water and/or energy networks design although it is performing and particularly adapted to these problems containing binary variables where very few integer solutions exist in the feasible region. Indeed, usually with a branch-and-Bound methodology, the resolution of an MINLP or MILP problem is very fastidious, and especially with water network design, because the binary variables control the solution. Consequently, the size of the tree with traditional methods becomes very large and the program often returns an infeasible error message before finding a solution. In this study, goal programming methodology has been successfully applied to the problem of water and/or energy network design. Its effectiveness has been successfully demonstrated by comparing the results obtained with other research works where different multiobjective optimization methods are employed. On the two specific examples studied, namely, a traditional IWN and an IWN with energy, trade-off solutions are obtained and compared with other solutions. Moreover, in the latter case, different temperature freshwater sources are studied in order to study the influence of these in heat exchangers.

Since in Boix et al.[24] the authors employed a lexicographic methodology based on the ε-constraint method and subsequent selection by TOPSIS procedures, treating four objective functions could constraint the solution space to a few solutions within the Pareto front for the sake of solution times and practicality. On the other hand, solutions in this work are obtained within seconds, and several modifications to the case study can be studied with little difficulty. Nevertheless, the usefulness of a posteriori methods is not questioned if the totality of the Pareto front is desired. Additionally, several a priori methods can be used in order to accomplish this task, for example, goal programming coupled with stochastic algorithms.

Relative to the objective functions chosen in this study, it is important to say that other type of objective functions could be formulated to obtain other type of results. The inclusion of e.g. piping, heat exchanger, freshwater and regenerated cost can be of great utility.

■ APPENDIX

5.1. IWN Model Statement

From the aforementioned problem (section 3.2.1), a mathematical model can be formulated. In the majority of previous works, the problem is generally stated in terms of concentrations and total mass flows, giving birth to bilinear terms in model equations,[3] resulting in MINLP formulations. Nevertheless, an IWN allocation problem can be stated as an MILP by complying with (i) only one contaminant is present on the network; (ii) total mass flows and concentrations are formulated in terms of partial mass flows; and (iii) contaminant flow is neglected in comparison to water flow in concentration calculations (see Savelski and Bagajewicz[46] and Bagajewicz and Savelski[9]). Also, it is assumed that water losses at regeneration units are negligible. The mathematical model is stated as follows (note that the index c now denotes contaminant and w water).

Water mass balance around a process:

$$Finp_i^w = fw_i + \sum_{j \in P, j \neq i} fp_{j,i}^w + \sum_{r \in R} frp_{r,i}^w, \quad i \in P \tag{14}$$

$$Foutp_i^w = fd_i^w + \sum_{j \in P, j \neq i} fp_{i,j}^w + \sum_{r \in R} fpr_{i,r}^w, \quad i \in P \tag{15}$$

$$Finp_i^w = Foutp_i^w, \quad i \in P \tag{16}$$

Contaminant mass balance around a process:

$$Finp_i^c = \sum_{j \in P, j \neq i} fp_{j,i}^c + \sum_{r \in R} frp_{r,i}^c + M_i^c, \quad i \in P \tag{17}$$

$$Foutp_i^c = fd_i^c + \sum_{j \in P, j \neq i} fp_{i,j}^c + \sum_{r \in R} fpr_{i,r}^c, \quad i \in P \tag{18}$$

$$Finp_i^c = Foutp_i^c, \quad i \in P \tag{19}$$

Water mass balance around a regeneration unit:

$$Finr_r^w = \sum_{m \in R, m \neq r} fr_{m,r}^w + \sum_{i \in P} fpr_{i,r}^w, \quad r \in R \tag{20}$$

$$Foutr_r^w = \sum_{i \in P} frp_{r,i}^w + \sum_{m \in R, m \neq r} fr_{r,m}^w, \; r \in R \tag{21}$$

$$Finr_r^w = Foutr_r^w, \quad r \in R \tag{22}$$

Contaminant mass balance around a regeneration unit:

$$Finr_r^c = \sum_{m \in R, m \neq r} fr_{m,r}^c + \sum_{i \in P} fpr_{i,r}^c, \quad r \in R \tag{23}$$

$$Foutr_r^c = frd_r^c + \sum_{i\in P} frp_{r,i}^c + \sum_{m\in R, m\neq r} fr_{r,m}^c, \quad r \in R \tag{24}$$

$$Finr_r^c = Foutr_r^c, \quad r \in R \tag{25}$$

Process splitter equations:

$$fp_{i,j}^c - Cout_i^{\max} fp_{i,j}^w = Foutp_i^c - Cout_i^{\max} Foutp_i^w, \quad i, j \in P, \quad i \neq j \tag{26}$$

$$fpr_{i,r}^c - Cout_i^{\max} fpr_{i,r}^w = Foutp_i^c - Cout_i^{\max} Foutp_i^w, \quad i \in P, \quad r \in R \tag{27}$$

$$fd_i^c - Cout_i^{\max} fd_i^w = Foutp_i^c - Cout_i^{\max} Foutp_i^w, \quad i \in P \tag{28}$$

Regeneration unit splitter equations:

$$frp_{r,i}^c - C_r^{\text{out}} frp_{r,i}^w = Foutr_r^c - C_r^{\text{out}} Foutr_i^w, \quad i \in P, \quad r \in R \tag{29}$$

$$fr_{r,m}^c - C_r^{\text{out}} fr_{r,m}^w = Foutr_r^c - C_r^{\text{out}} Foutr_i^w, \quad r, m \in R, \quad r \in m \tag{30}$$

Operating constraints

$$Finp_i^c \leq Cin_i^{\max} Finp_i^w, \quad i \in P \tag{31}$$

$$Foutp_i^c \leq Cout_i^{\max} Foutp_i^w, \quad i \in P \tag{32}$$

$$Foutr_r^c = C_r^{\text{out}} Foutr_r^w, \quad r \in R \tag{33}$$

In the last group, eqs 31 and 32 stand for the maximum concentration allowed at inlet and outlet of each process, while eq 33 fixes the outlet concentration of contaminant at the outlet of the regeneration units.

In order to model the decision whether it exists connections between process units and/or regeneration units or not, disjunctions are added to the model, such as for a freshwater connection to a process:

$$\begin{bmatrix} yp_i \\ fw_i \geq \min f \\ fw_i \leq \max f \end{bmatrix} \vee \begin{bmatrix} yp_i \\ fw_i = 0 \end{bmatrix}, \quad i \in P \tag{34}$$

Disjunctions such as eq 34 are added to each decision involved in the IWN allocation problem, relative to connections between processes, regeneration units, processes, and regenerations units, regeneration units and processes and processes and the discharge. In order to solve this disjunctive programming model, a simple Big-M reformulation is employed to transform the latter into a solvable MILP model:

$$minf(yw_i) \leq fw_i \leq maxf(yw_i), \quad i \in P \tag{35}$$

$$minf(yp_{i,j}) \leq fp_{i,j}^w \leq maxf(yp_{i,j}), \quad i, j \in P \tag{36}$$

$$minf(yd_i) \leq fd_i^w \leq maxf(yd_i), \quad i \in P \tag{37}$$

$$\min f(ypr_{i,r}) \leq fpr_{i,r}^w \leq \max f(ypr_{i,r}), \quad i \in P, \quad r \in R \tag{38}$$

$$\min f(yrp_{r,i}) \leq frp_{r,i}^w \leq \max f(yrp_{r,i}), \quad i \in P, \quad r \in R \tag{39}$$

$$\min f(yr_{r,m}) \leq fr_{r,m}^w \leq \max f(yr_{r,m}), \quad r, m \in R, \quad r \in m \tag{40}$$

In eqs 35–40, yw_i, $yp_{i,j}$, yd_i, $ypr_{i,r}$, $yrp_{r,i}$, $yr_{r,m}$, $i, j \in P$, $r, m \in R$, $i \neq j$, $r \neq m$ are indeed binary variables.

5.2. Industrial Water and Energy Network Model Statement

The model for the current problem is made of eq 14–40 and the following, which represent the addition of energy balances in the network.

Energy balance around a process unit:

$$Cp^w (fw_i Tw + \sum_{j\in P, j\neq i} fp_{j,i}^w Tp_k + \sum_{r\in R} frp_{r,i}^w Tr_r) + (Qp_i^+ - Qp_i^-) = Cp^w Tp_i (fd_i^w + \sum_{j\in P, j\neq i} fp_{i,j}^w + \sum_{r\in R} fpr_{i,r}^w), \quad i \in P \tag{41}$$

Energy balance around a regeneration unit:

$$Cp^w (\sum_{m\in R, m\neq r} fr_{m,r}^w Tr_m + \sum_{i\in P} fpr_{i,r}^w Tp_i) + (Qr_r^+ - Qr_r^-) = Cp^w Tr_r (frd_r^w + \sum_{i\in P} frp_{r,i}^w + \sum_{m\in R, m\neq r} fr_{r,m}^w), \quad r \in R \tag{42}$$

Global energy balance around the discharge:

$$Cp^w (\sum_{i\in P} fd_i^w Tp_i) + (Qd^+ - Qd^-) = Td \sum_{i\in P} fw_i \tag{43}$$

In addition, the following equations are added in order to model the disjunction to actually place a heat exchanger in a process or not:

$$\min Q(yexp_i^+) \leq Qp_i^+ \leq \max Q(yexp_i^+), \quad i \in P \tag{44}$$

$$minQ(yexp_i^-) \leq Qp_i^- \leq maxQ(yexp_i^-), \quad i \in P \tag{45}$$

$$yexp_i^+ + yexp_i^- \leq 1, \quad i \in P \tag{46}$$

Equations 44–46 ensure that both positive and negative heats are between stipulated bounds. In addition, eq 46 assure that only cooling or heating is allowed, or neither. For regeneration units and the discharge, the disjunctions are modeled analogously.

Finally, it is important to highlight that boilers/heaters are modeled as processes without contaminant load and by prohibiting inlet connections different than freshwater to these processes.

Nomenclature

Latin Symbols

nf = number of objective functions
w = weighting vector
$\overline{z}$ = reference vector
z^v = Nadir vector
z^r = aspiration vector
v = dummy variable
d^+ = positive deviation
d^- = negative deviation
f^{norm} = normalized objective function
$f^{\min}$ = minimum value of the objective function

f^{max} = maximum relative value of the objective function
goal = goal vector
$goal^{norm}$ = normalized goal
A = decision matrix
R = ranking in TOPSIS methods
P = index set of processes
np = number of processes
R = index set of regeneration units
nr = number of regeneration units
C = index set of components
nc = number of components
M_c = contaminant load
Cin^{max} = maximum concentration allowed at inlet
$Cout^{max}$ = maximum concentration allowed at outlet
C^{out} = outlet concentration
minf = minimum flow rate allowed
minf = maximum flow rate allowed
yw = existence of freshwater input
yp = existence of flow between processes
yprs = existence of flow between a process and a regeneration unit
yr = existence of flow between regeneration units
yd = existence of flow to the discharge
Fin = inlet flow rate
Fout = outlet flow rate
Tp = operation temperature of a process
Tw = freshwater temperature
Td = discharge temperature
Tr = operating temperature of a regeneration unit
fmaxp = maximum allowed flow rate to a process
fmaxr = maximum allowed flow rate to a regeneration unit
minQ = minimum allowed duty of a heat exchanger
maxQ = maximum allowed duty of a heat exchanger
yexp = existence of a heat exchanger in a process
yexr = existence of a heat exchanger in a regeneration unit
yexd = Eexistence of a heat exchanger in the discharge
Qp = heat flow of a process
Qr = heat flow of a regeneration unit
Qd = heat flow of the discharge
fp = flow rate between processes
frp = flow rate between a regeneration unit and a process
fd = flow rate from a process to the discharge
fpr = flow rate between a process and a regeneration unit
fr = flow rate between regeneration units
frd = flow rate from a regeneration unit and the discharge

Greek Symbols

ρ = sufficiently small positive scalar
ε = upper bound of an objective function

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Notes

The authors declare no competing financial interest.

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