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Sustainable wastewater treatment plants design through multiobjective optimization

Juan I. Padrón-Páez[a], Sofía De-León Almaraz[b], Alicia Román-Martínez[a,*]

[a] Universidad Autónoma de San Luis Potosí, Facultad de Ciencias Químicas, Av. Dr. Manuel Nava No. 6, Zona Universitaria,78210, San Luis Potosí, S.L.P., Mexico
[b] Université de Toulouse, Laboratoire de Génie Chimique, U.M.R. 5503 CNRS/INP/UPS 4 allée Emile Monso, 31432, Toulouse Cedex 4, France

ABSTRACT

Nowadays, an adequate design of wastewater treatment plants taking into consideration all sustainability dimensions– economic, environmental and social- is fundamental. This can be achieved by implementing systematic methodologies where conceptual and mathematical tools can be used together. This contribution proposes a framework that uses total cost, consumed energy, and reclaimed wastewater as sustainability metrics. A mixed-integer nonlinear programming problem arises from a general superstructure for wastewater treatment plants. A case study from Mexico City is solved by a hybrid multiobjective optimization approach that combines lexicographic and ε-constraint methods. Solutions are provided in the form of a Pareto front. A modified technique for order of preference by similarity to ideal solution (M-TOPSIS) analysis is used as a multiple criteria decision-making tool to find the best trade-off solution. The optimal sustainable configuration resulted consists of three levels of treatment and 100% of treated water reuse.

Keywords:
Wastewater treatment plants
Socio-eco-efficient sustainability
Multiobjective optimization
Mixed-integer nonlinear programming problem
Modified technique for order of preference by similarity to ideal solution
Multiple criteria decision making

1. Introduction

Wastewater is the polluted water generated by different activities, namely, industrial and municipal. Wastewater treatment plants (WWTPs) allow removing contaminants in water to comply with water quality norms and regulations. The growing importance of respecting and disseminating environmental standards, as well as inefficiency of plants due to poor designs and practices, motivate a necessity for systematic tools for WWTPs designs (Galan and Grossmann, 1998). The goal of wastewater management is to establish environmental protection measures, while economic and social concerns are considered (Metcalf and Eddy et al., 2014). One of the main questions to be answered before designing/installing a WWTP is related to the cost of the best technology that fulfills the environmental regulations of the discharged water, as well as to promote community development and public acceptance. The decision maker tries to find the best option at the lowest cost, but the selection of the most appropriate WWTP is not only an economic issue since other criteria such as environmental and social aspects must be considered in the decision process (Molinos-Senante et al., 2014). The inclusion of a sustainability assessment covering its three dimensions (economic, environmental, and social) can lead to a better wastewater management. Several procedures have been proposed to design wastewater treatment plants or wastewater treatment networks, and most procedures are based upon the application of rules of thumb or heuristics.

In general, the used methods can be classified into two broad classes to get good designs of these systems: those based on conceptual approaches, and those based on mathematical programming (Bagajewicz, 2000). The methods included in the first group are approximate and cannot guarantee optimality. Conceptual Design (CD) is a set of disciplines that contribute to the identification of the optimal design layout and nominal operating conditions of industrial processes (Barzaghi et al., 2016). For instance, the Pinch method is often used as a CD approach for water or heat exchange network problems.

Due to the inability of conceptual approaches to effectively provide rigorous solutions to complex problems, for example, multiple contaminant problems, mathematical programming has increased since the 1980s, facing the challenges associated with the water/wastewater allocation planning (WAP[1]) or the WWTP design. The WAP can be defined as follows: Given a set of water

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* Corresponding author.
E-mail address: alicia.romanm@uaslp.mx (A. Román-Martínez).

[1] for water/wastewater reuse

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Nomenclature

MINLP	Mixed-integer nonlinear programming
WWTP	Wastewater treatment plant
BOD_5	Biochemical Oxygen Demand
TSS	Total Suspended Solids
TN	Total Nitrogen
TP	Total Phosphorus
ds	Discharge stream
dc	Services to the public with direct contact
ic	Services to the public with indirect or occasional contact
i	Input stream
o	Output stream
j	Contaminant
m	Mixer
s	Splitter
h	Treatment units
k	Treatment levels
r	Purpose of reuse
osr	Self-recycle stream in the output
isr	Self-recycle stream in the input
irs	Recirculate stream towards the input
ors	Recirculate stream from the output
oby	Bypass stream from the output
iby	Bypass stream towards the input
dj	Disjunctions
A	Rivers are the discharge receptor bodies
B	Coastal waters are the discharge receptor bodies
C	Natural water deposits for the protection of aquatic life are the discharge receptor bodies
M	Number of Mixers
S	Number of splitters
TU	Number of the treatment units
TL	Number of the treatment levels
P-T	Pre-treatment
PT	Primary treatment
ST	Secondary treatment
TT	Tertiary treatment
$pmax_{j,\,h,\,k}$	Maximum percentage of removal reported of contaminant *j* for treatment *h* in the treatment level *k*
$E_{j,\,h,\,k}$	Removal efficiency coefficient of contaminant *j* for the treatment unit *h* in the treatment level *k*
$c_{j,\,ds}$	Concentration of contaminant *j* in the possible discharge streams *ds*
$c_{j,\,dc}$	Concentration of contaminant *j* in the possible reuse *dc*
$c_{j,\,ic}$	Concentration of contaminant *j* in the possible reuse *ic*
TC	Total cost
RE	Removal efficiency of pollutants
CE	Consumed energy
WR	Percent of reused water
$CC_{h,\,k}(F_{h,\,k})$	Function of the capital costs of treatment unit *h* for treatment level *k*
$OC_{h,\,k}(F_{h,\,k})$	Function of the operating costs of treatment unit *h* for treatment level *k*
$F_{h,\,k}$	Wastewater flowrate of treatment unit *h* at treatment level *k*
$c_{j,in}$	Concentration of contaminant *j* in the input
$c_{j,\,out}$	Concentration of contaminant *j* in the output
η_j	Removal efficiency for contaminant *j*
W_j	Weight associated for a specific pollutant *j*
$CE_{h,\,k}$	Proportion of the amount of consumed energy by the treatment unit *h* in treatment level *k*
F_r	Flowrate of treated wastewater reused for the purpose *r*
F_t	Total wastewater flowrate to be treated
F_k^{isr}	Flowrate of the self-recycle stream in the input *isr* for the treatment level *k*
F_k^{osr}	Flowrate of the self-recycle stream in the output *osr* for the treatment level *k*
F_{k-1}^{irs}	Flowrate of the recirculate stream towards the input *irs* for the stage $k-1$
F_k^{ors}	Flowrate of the recirculate stream from the output *ors* for the stage *k*
F_k^{oby}	Flowrate of the bypass stream from the output *oby* for the treatment level *k*
F_{k+2}^{iby}	Flowrate of the bypass stream towards the input *iby* for the treatment level $k+2$
$Y_{h,\,k}$	Binary variable used to choose treatment *h* for each treatment level *k*
Y_r	Binary variables utilized to select the type of reuse *r*
Y_{ds}	Binary variables utilized to select the type of receptor body *ds*
$Y_{sr,\,k}$	Binary variable used to restrict the existence of self-recycles streams
$Y_{by.k}$	Binary variable used to restrict the existence of bypass stream
$Y_{rs,\,k}$	Binary variable utilized to restrict the existence of recirculate stream
Y_{dj}	Binary variables for disjunctions
F_m^i	Flowrate of the input stream *i* for the mixer unit *m*
F_m^o	Flowrate of the output stream *o* for the mixer unit *m*
F_s^i	Flowrate of the input stream *i* for the splitter unit *s*
F_s^o	Flowrate of the output stream *o* for the splitter unit *s*
$F_{h,k}^i$	Wastewater flowrate in the input stream *i* of treatment unit *h* at treatment level *k*
$F_{h,k}^o$	Wastewater flowrate in the output stream *o* of treatment unit *h* at treatment level *k*
F_{ww}	Flowrate in the treatment units and/or treated wastewater effluents for the disjunctions
$c_{j,m}^i$	Concentration of the contaminant *j* in the input stream *i* for the mixer unit *m*
$c_{j,m}^o$	Concentration of the contaminant *j* in the output stream *o* for the mixer unit *m*
$c_{j,s}^i$	Concentration of the contaminant *j* in the input stream *i* for the splitter unit *s*
$c_{j,s}^o$	Concentration of the contaminant *j* in the output stream *o* for the splitter unit *s*
$c_{j,h,k}^i$	Concentration of contaminant*j* at the input *i* of treatment unit *h* for treatment level *k*
$c_{j,h,k}^o$	Concentration of contaminant *j* at the output *o* of treatment unit *h* for treatment level *k*

using units, a set of freshwater sources with corresponding contaminant concentrations, potential intermediate regeneration processes and a wastewater treatment units, one wants to obtain a water / wastewater-reuse / regeneration network that optimizes a given objective or objectives with any discharged water meeting the environmental regulations of concentration for each pollutant

(Bagajewicz and Faria, 2009). This work focuses on the study of systems of wastewater treatment, although there is a very close relationship between the study of allocation systems for freshwater and wastewater.

Even though the conceptual design approach has shown limitations, it is able to provide a simplified description of the problem, which can help to improve the formulation of the mathematical programming models. The mathematical approach has shown effectiveness in solving WAP problems, and the definition of the superstructure used can be very generic. Therefore, an approach that combines conceptual and mathematical programming approaches, seems to be a more effective alternative to face the challenges associated with the WAP or the WWTP design. In this regard, Statyukha et al. (2008) addressed the design of wastewater treatment network. The sequential strategy employed the water pinch analysis (CD approach) to develop a superstructure, and in the mathematical programming stage, the cost of the treatment process was minimized for the nonlinear programming (NLP) model. Also, Quaglia et al. (2014) proposed a framework for the design of wastewater treatment and reuse networks. The framework considered engineering knowledge, problem analysis tools, and optimization methods within a computer-aided environment. Sueviriyapan et al. (2016) extended the aforementioned work, focusing on the systematic design of a water management system for retrofit wastewater treatment networks of an existing industrial process, where the total annualized cost and the wastewater discharge rate were minimized. Besides, Castillo et al. (2016) presented an integrated framework for the optimal network selection of a WWTP configuration. The integrated methodology combines a knowledge-based technique and superstructure-based optimization (minimizing the total annualized cost). According to the authors, there is a mutual benefit and synergy achieved when both tools are integrated. Most of the works listed before cover the superstructure definition gap by using a two-step methodology. However, it has been detected a need for an integrated approach that ensures the right implementation of problem formulation and data collection for the adequate creation of a superstructure that gathers all feasible alternatives for real applications.

Regardless the available approaches used for designing treatment plants, the goal of sustainable development must be addressed, which is defined as “the development that meets the needs of the present generation without compromising the ability of future generations to meet their own needs” (WCED, 1987). Thus, the multidimensional nature of sustainability is fundamental and considers three dimensions. Nevertheless, some studies in the literature attempt to capture the sustainability requirements using a single indicator, e.g., through economic analysis (Balkema et al., 2002; Muga and Mihelcic, 2008). Most studies focus on the environmental and/or economic dimensions, ignoring the social aspects (Molinos-Senante et al., 2014). The multidimensional character of sustainability makes the selection of sustainable wastewater treatment systems a multiobjective optimization problem. However, in previous works, the sustainable design of wastewater treatment networks was not assessed completely, where the objective functions were related to the structure of the WWTP, its economic dimension of sustainability and very few considered environmental aspects such as energy consumption. To the best of our knowledge the social criterion has not been analyzed in multiobjective optimization approaches for WWTPs design. For instance, Rezaei et al. (2019) proposed a multiobjective optimization model for wastewater systems management, where the mathematical formulation consisted of two objective functions. The first objective function minimized the costs and incorporates a term that considered as a social indicator the price or the value of resource recovery. The second objective function minimized the greenhouse gas emissions (as an environmental indicator) of the wastewater system.

In that context, the aim of this work is to propose and validate a novel integrated approach for designing sustainable WWTPs for a multipollutant problem by multiobjective optimization. The analysis of the dedicated literature shows that a robust approach that can take into account a systematic approach to ensure the right data treatment, problem definition and multiobjective optimization by including the social aspect of sustainability is still missing, thus hampering the development of a generic approach. Therefore, the objective of this paper is twofold: 1) to develop a systematic framework to improve the problem definition, data gathering and superstructure definition of WWTPs (heuristic rules) and; 2) to propose a new multiobjective mathematical model that considers the three dimensions of sustainability. Therefore, our framework includes a combination of conceptual and mathematical programming approaches and proposes a six-step sequential methodology, indicating in each step its corresponding methods and tools, emphasizing all the substeps for an adequate mathematical programing model formulation and the integrated solution techniques (MINLP algorithms, lexicographic and ε-constraint method), to obtain a Pareto front solution, and, instead of allowing an informal or arbitrary WWTP selection from the Pareto front, the use of a multiple-criteria decision making (MCDM) method to find the best trade-off solution. This will be supported by a case study of a municipal WWTP from México City used for agricultural irrigation in the Valley of Tula (Mezquital Valley).

The remainder of this paper is organized as follows: Section 2 is devoted to present the general framework for the multiobjective design of sustainable WWTPs, where its methodological steps and sub-steps are explained. Section 3 is dedicated to the application of the framework through a real case study, showing the results and their analysis. Finally, in Section 4 the conclusions are given.

2. General framework and methodology

The problem of optimal design of sustainable WWTPs can be defined as a grassroot design, i.e., the design of a new process from scratch. Therefore, the wastewater streams with their respective contaminants, and different wastewater discharge effluents (or treated wastewater streams that can be reused) at a level of pollution established by environmental laws, are considered. From this information, the best design for a WWTP is obtained when it is evaluated with the sustainability criteria selected. The WWTP design includes the treatment technologies used, as well as the treated flowrates, the configuration of the process, and the flowrates of the streams of the treated wastewater for the different discharge types or reuse opportunities.

To solve the described WWTP design problem, the proposed framework is based on the generation, evaluation and selection of configurations and technologies (physical, chemical and/or biological), using a superstructure (which includes all process options), to identify the different stages of treatment, in terms of sustainability metrics. In Fig. 1, the flowchart of the proposed framework is shown, which is an iterative process, where sometimes it is necessary to return to one or more steps if a subsequent step cannot be completed. The integrated approach considers ruling out in advance those options that do not meet the different heuristic rules and restrictions, allowing a reduction of the search space before solving the optimization problem.

2.1. Step 1: Information/data collection and identification of bottlenecks

The aim of this step is to gather all the required data about the system under study. To create a database, relevant information for

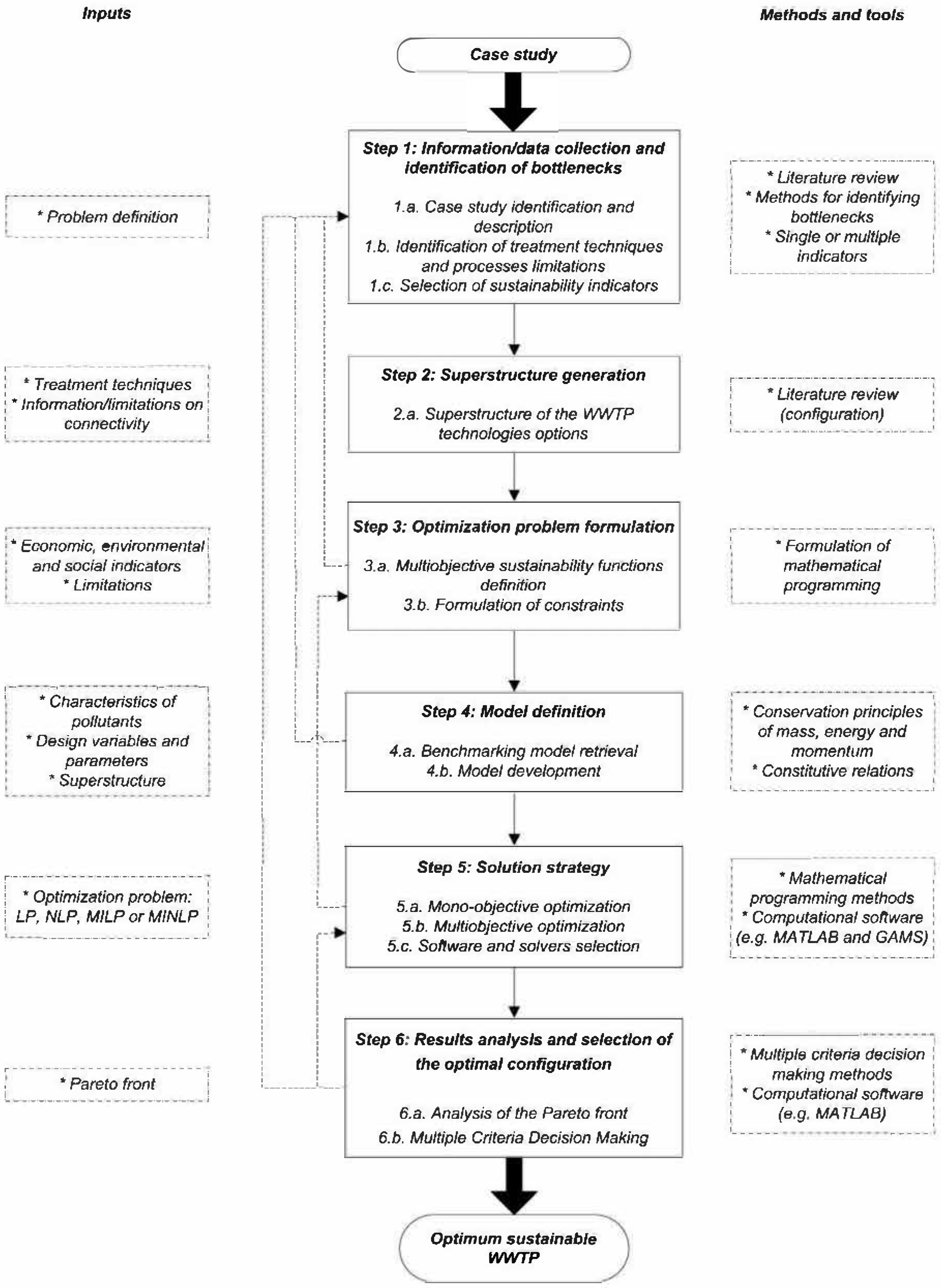

Fig. 1. Flowchart of the framework of sustainable WWTPs design.

the WWTP design must be investigated/collected, such as allowed types of treatment units, limits of contaminants, and wastewater discharge effluents.

2.1.1. Step 1.a. Case study identification and description

The necessary information to describe the system is: sources of wastewater (municipal and/or industrial), streams flowrates, wastewater characteristics, and treated wastewater effluents (discharge and reuse).

2.1.2. Step 1.b. Identification of treatment techniques and process limitations

Important factors that must be considered when evaluating and selecting a treatment technique are process applicability, influent wastewater characteristics, reaction kinetics, treatment contaminants capability, operating parameters, maintenance requirements, chemical requirements, and complexity. On the other hand, methods for identifying bottlenecks are based on experiments, heuristic and/or simulations (Ben-Guang et al., 2000). In this methodology, a combined heuristic or knowledge-based approach and simulations are employed.

2.1.3. Step 1.c. Selection of sustainability indicators

It is important to determine the economic, environmental, and social factors that allow evaluating and selecting the best technologies for wastewater treatment. Therefore, a critical review of potential sustainability metrics is carried out. For the economic aspect, most analysis encompasses financial costs and benefits (Balkema et al., 2002; Muga and Mihelcic; 2008; Molinos-Senante et al., 2014). Environmental dimension refers to the ability of the natural world to withstand the impact of human activity (Popovic et al., 2013). Some of the most used ones are contaminants removal efficiency, energy consumption, and emissions (Balkema et al., 2002; Muga and Mihelcic; 2008; Molinos-Senante et al., 2014). According to Balkema et al. (2002), the purpose of the social aspect is to secure people's socio-cultural and spiritual needs in an equitable way. This criterion can be assessed by quantitative and qualitative indicators. Some possible options include the percentage of wastewater reused and community size served (Popovic et al., 2014). The possible sustainability metrics arise by identifying the requirements of the system through the bottleneck analysis.

2.2. Step 2: Superstructure generation

In this step, the possible configurations arose from step 1, and their combinations among different equipment and their connection streams that may constitute the WWTP are generated. The centralized, decentralized schemes and several variations of these (e.g., distributed), which are the most commonly used configurations (Bagajewicz, 2000) are considered.

2.2.1. Step 2.a. Superstructure of the WWTP technologies options

Generally, four stages can be distinguished: pre-treatment, primary treatment, secondary treatment, and tertiary treatment. Historically, pre-treatment and primary treatment levels have been linked to physical methods; the secondary treatment has been associated with chemical or biological techniques, and for tertiary treatment, it has been considered a combination of methods. The most appropriate techniques (for each stage) that potentially allow carry out the treatment process efficiently are selected from step 1.b. Table 1 shows comparisons among different treatment techniques to aid in the options generation and in the identification of limitations.

2.3. Step 3: Optimization problem formulation

At this stage, the objective functions in terms of sustainable criteria along with the constraints, are defined. The sustainable design of WWTP can be formulated as a multiobjective optimization problem and has the following general form:

$$\begin{aligned}
&Min\ [f_1(x,y), f_2(x,y), \ldots, f_k(x,y)]\\
&g(x,y) \le 0\\
&h(x,y) = 0\\
&x \in X\\
&y \in Y
\end{aligned} \tag{1}$$

where x is a vector of m continuous variables, y is a vector of n nonnegative integer variables ($Y \in \mathbb{Z}^n_{\ge 0}$), $h(x,\ y)$ are p equality constraints, $g(x,\ y)$ are q inequality constraints, and $f_i(i = 1, \ldots, k)$ is a function where $\mathbb{R}^m \times \mathbb{Z}^n_{\ge 0}$ on $\mathbb{R}$, $h(x,y) \in \mathbb{R}^p$, $g(x,y) \in \mathbb{R}^q$ and $X \in \mathbb{R}^m$ (Collette and Siarry, 2003). The continuous variables define process variables (flowrates, the concentration of contaminants, etc.), and integer variables are used to model sequences of events, existence (or non-existence) of processing units and connectivity among techniques are represented by binary variables.

2.3.1. Step 3.a. Multiobjective sustainability functions definition

From the indicators of step 1.c., the functions that consider the most significant aspects of sustainability are formulated as mathematical functions. In the context of mathematical programming, cost functions are the most common. Regarding the environmental criteria, indicators can be formulated as an individual objective or as a sum of individual objectives; for example, through life cycle analysis (Padrón-Páez et al., 2017). The majority of social metrics are of a qualitative nature, but the use of quantitative indicators facilitates the representation of an objective function associated with the social dimension. For simplicity, the criteria selection depends to a large extent on the availability of information.

2.3.2. Step 3.b. Formulation of constraints

In general, constraints are classified as equality and inequality ones. Different kinds of constraints are involved in this work: the process model, logical, structural, and operational constraints. The process model is a set of equality constraints that represent the mass and energy balance equations, which describe the behavior of the process. Logical constraints represent the selection of equipment and the sequence of operations in the processing steps. The structural constraints define the connectivity between unit operations. Operational constraints are related to process operative specifications, such as the flowrate of treated wastewater. The process model is developed in step four of the framework. When it is not possible to determine the objective functions and restrictions or if there is not enough information about them, returning to step 1 must be considered.

2.4. Step 4: Model definition

The goal of this step is to develop the mathematical model that represents the given case study, that is, the set of equations for the process units and their respective compounds involved.

2.4.1. Step 4.a. Benchmarking model retrieval

Constitutive models are related to the terms that require definition or calculation in the conservation equations of mass, energy, and momentum. Thus, it is possible to search in a library of models to select those that are suitable for the optimization problem.

2.4.2. Step 4.b. Model development

The model equations can be developed through a modeling tool using a systematic procedure. One option is to apply the seven-step modeling procedure proposed by Hangos and Cameron (2001). Another possibility is to follow standard relations, as in the models proposed for optimization purposes (Galan and Grossmann, 1998; Padrón-Páez et al., 2017). In this step, it is possible to find out that there are neither suitable constitutive relations in the literature nor information about parameters values of the model. This situation could make us reconsider going back to step 1.

2.5. Step 5: Solution strategy

In this step, the suitable optimization strategy for mono-objective and multiobjective frameworks is selected. Thus, relevant aspects of the optimization problem are analyzed, such as linearity, convexity, and variable types. Once the methods to solve the

Table 1
Comparative analysis of the advantages and disadvantages of some wastewater treatment techniques.

Treatment Techniques	Capability to treat contaminants	Operating parameters and/or design variables	Advantages	Disadvantages
Screening	* Biochemical Oxygen Demand (BOD5) * Suspended solids (coarse solids)	* Bar size (width and depth) * Clear spacing between bars * Slope from vertical * Approach velocity * Allowable head loss	* Protects equipment from subsequent processes * Easy to operate * High wastewater flowrate can be treated	* Emissions of volatile compounds * A lot of maintenance required (obstruction) * Low efficiency removal * Waste sludge is produced
Primary sedimentation	* Biochemical Oxygen Demand (BOD5) * Suspended solids * Heavy metals	* Detention time * Surface loading rates * Weir loading rate * Scour velocity * Type, size and shape of the tanks	* Removal of large particles * Protects equipment from subsequent processes * Easy to operate	* Emissions of volatile compounds * Inadequate for light solids and stable emulsions * Waste sludge is produced * Chemical agents may be required
Aerobic processes	* Removal of organic compounds (BOD5) * Removal of nutrients (nitrogen and phosphorus)	* Dissolved oxygen concentration * Process kinetics (rate expression) * Kinetic parameters (reaction rate constant) * Reactor volume * Residence time * Solids retention time and loading * Mass transfer coefficient in aeration process (k_La) * Temperature	* Removal of dissolved pollutants * Destruction process * Low maintenance required * Relatively easy to operate * Low capital costs * High wastewater flowrate can be treated	* Emission of volatile compounds * Waste sludge is produced * Susceptible to changes in load and toxins * Susceptible to climate changes * High residence time
Anaerobic processes	* Removal of organic compounds (BOD5)	* Process kinetics (rate expression) * Kinetic parameters (reaction rate constant) * Reactor volume * Organic loading rate * Solids retention time * Residence time * Temperature	* Removal of dissolved pollutants * Destruction process * Produces methane * Reduces the generation of waste sludge	* Susceptible to changes in load and toxins * Susceptible to climate changes * Capital and operational costs relatively high * Moderate removal efficiency (<85%) * High residence time (greater than the aerobic process)
Processes with membranes	* Removal of organic (BOD5) and inorganic compounds (e.g. heavy metals) * Removal of suspended solids and microorganisms (e.g. bacteria)	* Pore size * Operating pressure * Minimum particle size removed * Membrane materials * Membrane configuration	* Removal of dissolved constituents * Metal recovery * Easy to operate * It can be used to separate waste sludge * Wastewater can be reused	* Removal efficiency varies with the membrane material used * The retained solid in the membrane must be disposed * Chemical additives may be required (e.g. coagulants) * Selective removal * Complicated maintenance * Membrane fouling

mono and multi-objective problems are defined, the available computational software is analyzed for the implementation of the optimization strategies through the software library solvers.

2.5.1. Step 5.a. mono-objective optimization

Based on linearity (or nonlinearity) and the decision variables (continuous and/or integers) the optimal design of WWTP can be formulated as linear programming (LP), nonlinear programming (NLP), mixed-integer linear programming (MILP), or mixed-integer nonlinear programming (MINLP). A comparative analysis of the solution algorithms is carried out to choose the most appropriate method depending on the optimization problem (Edgar et al., 2001).

2.5.2. Step 5.b. Multiobjective optimization

In these methods, the concept of optimality is changed by Pareto optimality. Thus, the solutions that cannot be improved in one objective function without deteriorating their performance in at least one of the others are non-dominated solutions (Collette and Siarry, 2003). The multiobjective optimization methods can be classified into three groups, *a priori, a posteriori* and hybrid methods (De-León Almaraz, 2014). In an analogous manner to step 5.a., a comparative analysis is done to select the most appropriate method that allows obtaining the non-dominated solutions.

2.5.3. Step 5.c. Software and solvers selection

To solve the optimization problem formulated in previous steps, the solution strategies that were chosen are implemented in adequate computational software. GAMS is probably one of the most used computational software to solve mathematical programming models, but there are other alternatives, such as the MATLAB® optimization toolbox. The decision guidelines about the use of computational software, among other factors, are based on the availability of the computational software itself and the user's knowledge. If it is not possible to obtain feasible solutions of the optimization problem or the set of optimal solutions is not satisfactory, it must be considered going back to step 3 to evaluate the selection of objective functions or constraints.

2.6. Step 6: Results analysis and selection of the optimal configuration

The implementation and solution of a multiobjective optimization strategy lead to a set of optimal trade-off solutions (Pareto front) that satisfy the objective functions to the best possible extent. Therefore, the decision maker's task is now to select the best choice among the optimal trade-off solutions. In order to guide this decision, the use multiple criteria decision making (MCDM) tool is proposed.

2.6.1. Step 6.a. Analysis of the pareto front

The solutions represented in the Pareto front correspond to the different optimal design strategies for the WWTP in the associated variable space.

2.6.2. Step 6.b. Multiple criteria decision making

In general, it is not possible to specify which of the optimal solutions is the best trade-off solution because they all satisfy the Pareto optimality condition. Instead of allowing an informal or arbitrary WWTP selection from the Pareto front, this paper proposes the use of multiple-criteria decision making (MCDM) methods to find the best trade-off solution. MCDM refers to all methods that aid people to make decisions according to their preferences, in cases where there are more than one conflicting criteria (Mardani et al., 2015). These methods allow choosing, sorting and arranging data sets (Collette and Siarry, 2003). A review of the applications and methodologies of the MCDM techniques and approaches can be found in Mardani et al. (2015). Some of the existing methods are ELECTRE, TOPSIS, and AHP, which can be applied in supply chain, safety and risk management, energy, environment, sustainability, and other fields.

The selection of the MCDM method is mainly based on the applicability of the technique for a given problem. A variety of methods exists. ELECTRE (Elimination and Choice Translating Reality) method was introduced by Roy (1968) developed to deal with "outranking relations" by using pair wise comparisons among alternatives under each one of the criteria separately. This method is especially convenient when there are decision problems that involve a few criteria with many alternatives saving time. A very popular MCDM is TOPSIS (Technique for Order Preference by Similarly to Ideal Solution) developed by Hwang and Yoon (1981) as an alternative to ELECTRE. The basic concept of TOPSIS is that the chosen alternative should have the shortest distance from the positive ideal solution (utopia point) and the furthest from the negative ideal solution (nadir point). The relative distance from each evaluated alternative to the ideal reference point is calculated to determine the ranking order of all alternatives (Ren et al., 2007). This approach offers several advantages: rational and understandable; simple calculation, the concept permits the pursuit of the best alternatives for each criterion depicted in a simple mathematical form and, the importance weights are incorporated into the comparison procedures. However, one of the problems related to TOPSIS is that it can cause the phenomenon known as rank reversal (García-Cascales and Lamata, 2012). In this phenomenon, the alternative order of preference changes when an alternative is added to or removed from the decision problem. To deal with this problem, the method M-TOPSIS, developed by Ren et al. (2007) was proposed as a novel, modified TOPSIS (M-TOPSIS) method to evaluate the quality of the alternative and to deal the rank reversal problem. For this reason, M-TOPSIS method has been used for the proposed framework in this work.

If not enough optimal solutions are obtained to analyze the Pareto front from its shape, it is considered returning to step 5. Additionally, in case of any inconsistency is found, it is recommended to check for errors in the solution algorithm used for the optimization problem. On the other hand, if the selection of the optimal process does not meet the preferences of the decision makers, it is considered to return to step 1. Note that the optimal WWTP is difficult to obtain in one pass through the framework proposed. Therefore, some iterations are needed.

3. Application of the framework

In this section, the framework presented for the optimal design of sustainable WWTP is applied to a case study, which addresses the problem of municipal wastewater treatment. The case study is based on data available in the literature and aims at representing the complexity of a municipal WWTP grassroot design, which is related to the quantity and type of contaminants, the number of treatment techniques options, the compliance of environmental regulations, and the sustainable water management. The problem statement can be defined as: given a set of streams from the municipal sewage with known flowrates, that contains certain pollutants with known concentrations and different wastewater discharge effluents or streams of treated wastewater for reuse; the goal is to design a WWTP that can remove a load of pollutants to desired limits (standards) for discharge and/or reuse, that best fulfill the sustainability functions. It is expected to get the best design in terms of sustainability, the output results must be the treatment technologies used and the treated flowrates, the configuration of the process, and the flowrates streams of the treated wastewater for discharge or reuse. In the following subsections, the formulation and solution of a case study for a sustainable WWTP grassroot design problem, according to the proposed framework, is displayed.

3.1. Step 1: Information/data collection and identification of bottlenecks

3.1.1. Step 1.a. Case study identification and description

A municipal wastewater case from Mexico City used for agricultural irrigation in the Valley of Tula, known as the Mezquital Valley, is considered (Jiménez, 2005). Mexico City generates an average of 75 m^3/s of wastewater (municipal), which is collected in a unified combined sewer system. The wastewater must be treated before discharge to meet the environmental limits established by the Mexican Official Standards (SEMARNAT, 2014). In this case, the metals concentrations are within the allowable limits. Then, we are focusing on treating the contaminants of concern in terms of the biochemical oxygen demand (BOD_5), total suspended solids (TSS), total nitrogen (TN) and total phosphorus (TP). Table 2 shows the average characteristics of this wastewater, as well as the permissible limits of discharges. Thus, three types of receptor bodies are considered A, B, and C. For type A, rivers are the receptor body; coastal waters are considered for type B, and type C considers natural water deposits for the protection of aquatic life. Regarding the reclaimed water, two possible types of reuses for treated water are considered: services to the public with direct contact (DC) and services to the public with indirect or occasional contact (IC). The selection of the wastewater discharge effluents and the purposes of reuse are based on the environmental standards established by SEMARNAT (2014). This information suggests that the configuration of the WWTP may have more than one discharge stream.

3.1.2. Step 1.b. Identification of treatment techniques and processes limitations

A comprehensive review of the available information in the literature was carried out concerning contaminants and treatment techniques (Brinkmann et al., 2016; Hendricks, 2006; Metcalf and Eddy et al., 2014; Romero, 2004). This information was analyzed according to heuristic methods utilized for identifying bottlenecks, to rule out those techniques that are not capable of removing the contaminants in the influent for the case study and/or are not suitable to accomplish the goals of the treatment in the WWTP. Additionally, the selection of treatment techniques depends on the availability and quality of the data. Then, the considered techniques are screening, grit separator, oil-water separation, primary

Table 2
Characteristics of Mexico City's wastewater and discharge limits (SEMARNAT, 2014) (Receptor bodies, A: rivers; B: coastal waters; C: Natural water deposits for the protection of aquatic life).

Contaminant (mg/l)	Average	Receptor body A limits	Receptor body B limits	Receptor body C limits	Services with direct contact limits	Services with indirect contact limits
BOD_5	240	200	150	60	20	30
TSS	295	200	125	60	20	30
TN	26	60	60	25	60	60
TP	10	30	30	10	30	30

Table 3
Capital cost and Operating cost for techniques of the WWTP options.

Treatment unit or combination	Capital cost (*USD*)	Operating cost (*USD/year*)	Reference
Screening	$196F^{0.56}$	$0.0215F^{0.4398}$ ***	Romero-Rojas, 2004 Martin and Martin, 1991
Grit separator	$123F^{0.76}$	$0.0215F^{0.4398}$ ***	
Oil-water separation	$4,800F^{0.7*}$	$0.0215F^{0.4398}$ ***	Kuo and Smith, 1997 Martin and Martin, 1991
Primary sedimentation	$375F^{0.7}$	$11.02F^{1.01}$	Romero-Rojas, 2004
Filtration	$1,405F^{0.61}$	$11.02F^{1.01}$	
Flotation	$29,837F^{0.37}$	$842.4F^{0.6135}$	Brinkmann et al., 2016
Coagulation/flocculation+Primary sedimentation	$375F^{0.7} + 30F^{0.91}$	$11.02F^{1.01}$	Romero-Rojas, 2004
Aerobic processes	$72F + 368,043$	$4.58F + 36,295$	Qasim, 1998
Anaerobic processes	$11,512F^{0.4526}$	$0.67F + 26,748$	
Aerobic + anaerobic process	$72F + 368,043$ $+11,512F^{0.4526}$	$5.25F + 63,043$	
Anaerobic + anoxic + aerobic processes combined	$162F + 980,820$ $+11,512F^{0.4526}$	$93F^{0.834} + 5.25F$ $+63,043$	
Chemical oxidation	$121,204F^{0.3767}$	$1,287.4F$	Brinkmann et al., 2016
Chemical precipitation***	$0.0488F + 0.0218$	$0.0265F + 0.0218$	Martin and Martin, 1991
Membrane processes **	$70.419F^{0.749}$	$265.97F^{0.5429}$	Sharma, 2010
Carbon adsorption	$262.22F^{0.9367}$	$1,480.1F^{0.6076}$	Qasim, 1998
Ion exchange **	$1,074F^{0.445}$	$654.07F^{0.3878}$	Sharma, 2010
Stripping *	$16,800F^{0.7}$	$8,600F$	Kuo and Smith, 1997
Electrochemical processes	$73,073F^{0.2263}$	$0.48F^{1.44}$	Romero-Rojas, 2004 Brinkmann et al., 2016

Note: F in m^3/d, *F in t/h, ** F in gpd, *** F in MGD and its cost is generated in million dollars.

sedimentation, filtration, flotation, coagulation/flocculation combined with primary sedimentation, aerobic process, anaerobic process, aerobic combined with anaerobic process, anaerobic-anoxic-aerobic processes combined, chemical oxidation, chemical precipitation, membrane processes, carbon adsorption, ion exchange, stripping and electrochemical processes.

3.1.3. Step 1.c. Selection of sustainability indicators

From a literature review (Balkema et al., 2002; Molinos-Senante et al., 2014; Popovic et al., 2014), it was determined that total cost, removal efficiency of contaminants, energy consumption and customer value are the indicators that represent in a dependable way the three dimensions of sustainability (Tables 3-5). The total cost is the sum of capital costs (CAPEX) and operating costs (OPEX), which are considered to assess the economic aspect. The removal efficiency of contaminants and the energy consumption are proposed to cover the environmental aspect. The first environmental criterion is an indicator of the overall system efficiency. On the other hand, the energy consumption in the WWTP is an indicator to address optimal resource utilization (Balkema et al., 2002). For the social dimension of sustainability, an indicator to measure the customer value is proposed. This metric evaluates the amount of treated water that is reused and its purpose (Popovic et al., 2014). For example, reclaimed water for non-potable reuse purposes such as landscape irrigation. The use of reclaimed water is an indirect mode to measure public trust in wastewater facilities. Table 4

3.2. Step2: Superstructure generation

3.2.1. Step 2.a. Superstructure of the WWTP technologies options

A general superstructure for the connections between technologies and streams is proposed. From Fig. 2, it is possible to get the optimal configuration of a WWTP, considering splitting units (S), mixing units (M) and treatment units (TU). From the information collected and the analysis of limitations for the treatment techniques, the potential treatment units were determined for the different stages of the WWTP. The techniques for the first level are screening, grit separator, and oil-water separation. Primary treatment considers primary sedimentation, filtration, flotation and coagulation/flocculation combined with primary sedimentation. Aerobic process, anaerobic process, aerobic combined with anaerobic process, combined anaerobic-anoxic aerobic processes and chemical oxidation treatments are available at the secondary treatment stage. In the tertiary treatment, chemical precipitation, membrane processes, carbon adsorption, ion exchange, stripping and electrochemical processes are included.

3.3. Step 3: Optimization problem formulation

3.3.1. Step 3.a. Multiobjective sustainability function definition

Several criteria are considered simultaneously, which are related to the three dimensions of sustainability. From an economic perspective, the purpose of the multiobjective optimization is to minimize the total cost (TC) of the WWTP design.

$$Min\ TC = \sum_{k}^{TL} \sum_{h}^{TU} CC_{h,k}\left(F_{h,k}\right) + OC_{h,k}\left(F_{h,k}\right), \ \forall h \in TU, \ \forall\ k \in TL \quad (2)$$

Table 4
Removal efficiency for techniques of the WWTP options.

Treatment unit or combination	Removal efficiency (%)				
	BOD_5	TSS	TP	TN	Reference
Screening	0–5	5–10			Qasim, 1998
Grit separator	0–5	0–10			Romero-Rojas, 2004
Oil-water separation		50			Kuo and Smith, 1997
Primary sedimentation	30–40	50–65	10–20	20–40	Qasim, 1998
Filtration	20–60	60–80	20–50	50–70	
Flotation	10–50	70–95			Romero-Rojas, 2004
Coagulation/flocculation+ Primary sedimentation	40–70	50–80	70–90	50–90	Qasim, 1998
Aerobic processes	80–85	80–90	10–25	60–85	Qasim, 1998
Anaerobic processes	75–85				Metcalf and Eddy et al., 2014
Aerobic + anaerobic process	99				Brinkmann et al., 2016
Anaerobic + anoxic + aerobic processes combined	90–95	80–95	70–90	70–95	Qasim, 1998
Chemical oxidation	70–99			80–95	Brinkmann et al., 2016
Chemical precipitation	50–85	70–90			Romero-Rojas, 2004
Membrane processes	90–100	90–100	90–100	90–100	Qasim, 1998
Carbon adsorption	50–85	50–80	10–30	30–50	
Ion Exchange				90–95	
Stripping				60–95	
Electrochemical processes	85	95			Statyukha et al., 2008

Table 5
Consumed energy for techniques of the WWTP options.

Treatment unit or combination	Consumed energy (kWh/m^3)	References
Screening	0.0003–0.0005	Metcalf and Eddy et al., 2014
Grit separator	0.003–0.013	
Oil-water separation	0.06	Quaglia et al., 2014
Primary sedimentation	0.0057–0.0082	EPRI, 2013
Filtration	0.003	Persson et al., 2006
Flotation	0.03–0.04	Metcalf and Eddy et al., 2014
Coagulation/flocculation + primary sedimentation	0.0177–0.02	EPRI, 2013
Aerobic processes	0.13–0.32	Metcalf and Eddy et al., 2014
Anaerobic processes	0.093–0.16	
Aerobic + anaerobic process	0.6	Amiri et al., 2015
Anaerobic + anoxic + aerobic processes combined	0.503–0.57	Metcalf and Eddy et al., 2014 Molinos-Senante et al., 2014
Chemical oxidation	0.05–0.1	Metcalf and Eddy et al., 2014
Chemical precipitation	0.0002–0.0024	EPRI, 1996
Membrane processes	0.5–0.65	Metcalf and Eddy et al., 2014
Carbon adsorption	0.02–0.035	Mousel et al., 2017
Ion exchange	0.395	Drewes et al., 2009
Stripping	0.1–0.5	Brinkmann et al., 2016
Electrochemical processes	1.1–2.2	Metcalf and Eddy et al., 2014

where $CC_{h,\,k}(F_{h,\,k})$ and $OC_{h,\,k}(F_{h,\,k})$ are functions of the system flowrates that can take different forms, like linear, exponential, potential and polynomial (Table 2).

Two objective functions are proposed to cover the environmental aspect, the removal efficiency of contaminants (*RE*) and the consumed energy (*CE*). This last criterion can also be considered as an eco-efficient indicator (environmental and economic) (Álvarez del Castillo-Romo et al., 2018), since it influences the operational cost (OPEX) of a WWTP. The first environmental criterion is defined as the maximization of the sum of the global removal efficiency of contaminants:

$$Max\ RE = \sum^{J} \eta_j W_j,\ \ j = 1, 2, \ldots, J \tag{3}$$

where

$$\eta_j = \frac{c_{j,\ in} - c_{j,out}}{c_{j,in}} \tag{4}$$

where *RE* is the sum of the individual removal efficiency for each contaminant (η_j) multiplied by the weight associated for a specific pollutant (W_j), and η_j is defined from the initial and final concentrations of pollutants in the overall process ($c_{j,in}$ and $c_{j,\ out}$). The minimization of consumed energy (*CE*) in the WWTP is defined as:

$$Min\ CE = \sum_{k}^{TL} \sum_{h}^{TU} CE_{h,k} F_{h,k},\ \ \forall h \in TU,\ \ \forall\ k \in TL \tag{5}$$

where, *CE* is the summation of the individually consumed energy by the treatment units ($CE_{h,\,k}$) multiplied by the wastewater flowrate ($F_{h,\,k}$).

For the social dimension, the percent of water reused (*WR*) or the use of reclaimed water is maximized, using the following function:

$$Max\ WR = \left(\frac{\sum_{r}^{R} F_r}{F_t} \right) \times\ 100,\ \ r = 1, 2, \ldots,\ R \tag{6}$$

where, F_r is the flowrate of reused treated wastewater for the purpose *r*, and F_t is the total wastewater flowrate. The different purposes of reuse (DC and IC) are considered equally important, although relative weights can be used.

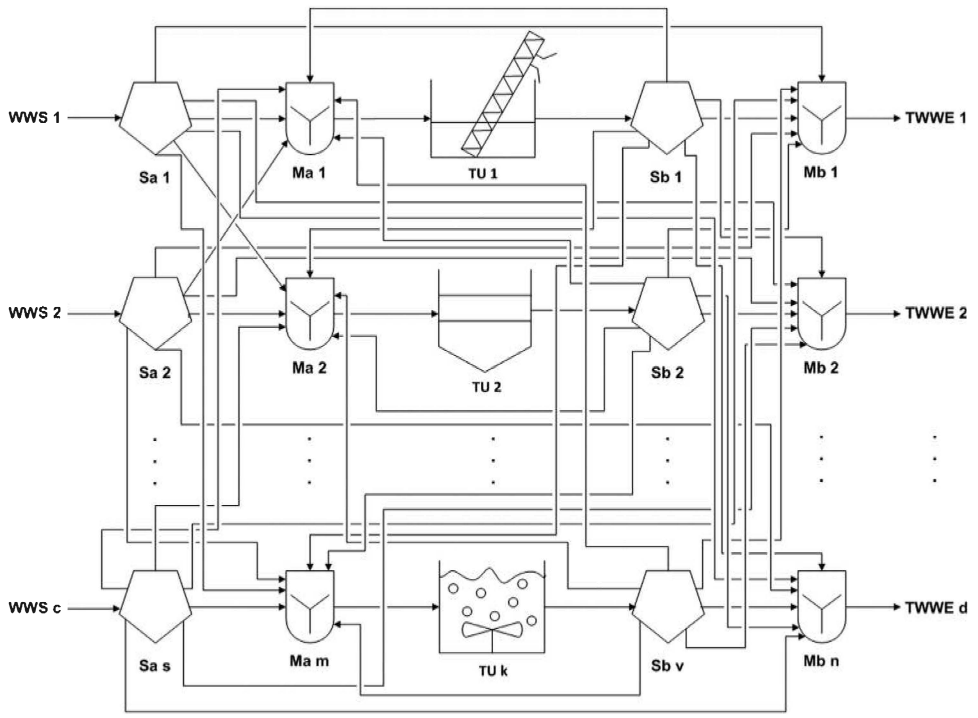

Fig. 2. General superstructure for a WWTP (*WWS*: Wastewater source, S_a and S_b: Splitters, M_a and M_b: Mixers, *TU*: Treatment units and *TWWE*: Treated wastewater effluents).

3.3.2. Step 3.b. Formulation of constraints

For the setting of logical constraints, it is only possible to select one treatment technique by stage Eq. (7)). Also, in the final discharge, three streams exit to two types of reuses (DC and IC). In addition, there is only a single type of receptor body (Eqs. (8) and (9).

$$\sum_{h}^{TU} Y_{h,k} \le 1, \ \forall k \in TL \tag{7}$$

$$\sum^{R} Y_r \le 2, \ r = 1,2 \tag{8}$$

$$\sum_{ds}^{DS} Y_{ds} \le 1, \ ds = 1,2,3 \tag{9}$$

where $Y_{h,\,k}$ are binary decision variables for the treatment h with the number of equipment *TU* for each treatment level k with the number of stages *TL* in the WWTP. The binary variables utilized to select the type of reuse (r) and the type of receptor body (ds) are Y_r and Y_{ds}, respectively. Additionally, a maximum of four treatment stages is defined:

$$\sum_{k}^{TL} \sum_{h}^{TU} Y_{h,k} \le 4, \ \forall h \in TU, \ \forall \ k \in TL \tag{10}$$

For structural constraints definition, recirculation to the same treatment unit is not allowed, because this would imply that the technique is inadequate for the treatment of the contaminants to be removed Eqs. (11) and ((12)):

$$F_k^{osr} Y_{sr,k} = F_k^{isr}, \ \forall k \in TL \tag{11}$$

$$\sum_{k}^{TL} Y_{sr,k} = 0, \ k = 1,2,3,4 \tag{12}$$

where $Y_{sr,\,k}$ are binary variables to restrict self-recycled streams. F_k^{osr} and F_k^{isr} are the flowrates of the self-recycle streams in the output and input, respectively.

In order to obtain appropriate characteristics of the wastewater to be treated at each level of the system, it is only possible to recirculate a stream to the previous stage of treatment (for example, from secondary treatment to primary treatment), and a stream cannot skip the sequential order of treatment for one or more stages of the WWTP (bypasses), given by the Eqs. (13), (14) and (15).

$$F_{k-1}^{irs} \ Y_{rs,k} = F_k^{ors}, \ k = 2,3,4 \tag{13}$$

$$F_k^{oby} = \sum_{k}^{2} F_{k+2}^{iby} \ Y_{by.k}, \ k = 1,2 \tag{14}$$

$$\sum_{k}^{2} Y_{by,k} = 0, \ k = 1,2 \tag{15}$$

where, F_{k-1}^{irs} is the flowrate of the recirculated stream towards the input, F_k^{ors} is the flowrate of the recirculated stream from the output, F_k^{oby} is the flowrate of the bypass stream from the output, F_{k+2}^{iby} is the flowrate of the bypass stream towards the input, $Y_{rs,\,k}$ and $Y_{by,k}$ are binary variables.

For the formulation of the operational constraints, the concentrations of pollutants in the discharge streams should meet environmental regulations, as well as the concentrations of contaminants for each type of reuse:

$$0 \le c_{j,ds} \le c_{j,ds}^{max}, \ \forall j \in J, \ \forall ds \in DS \tag{16}$$

$$0 \le c_{j,dc} \le c_{j,dc}^{max}, \ \forall j \in J, \ \forall dc \in DC \tag{17}$$

$$0 \le c_{j,ic} \le c_{j,ic}^{max}, \ \forall j \in J, \ \forall ic \in IC \tag{18}$$

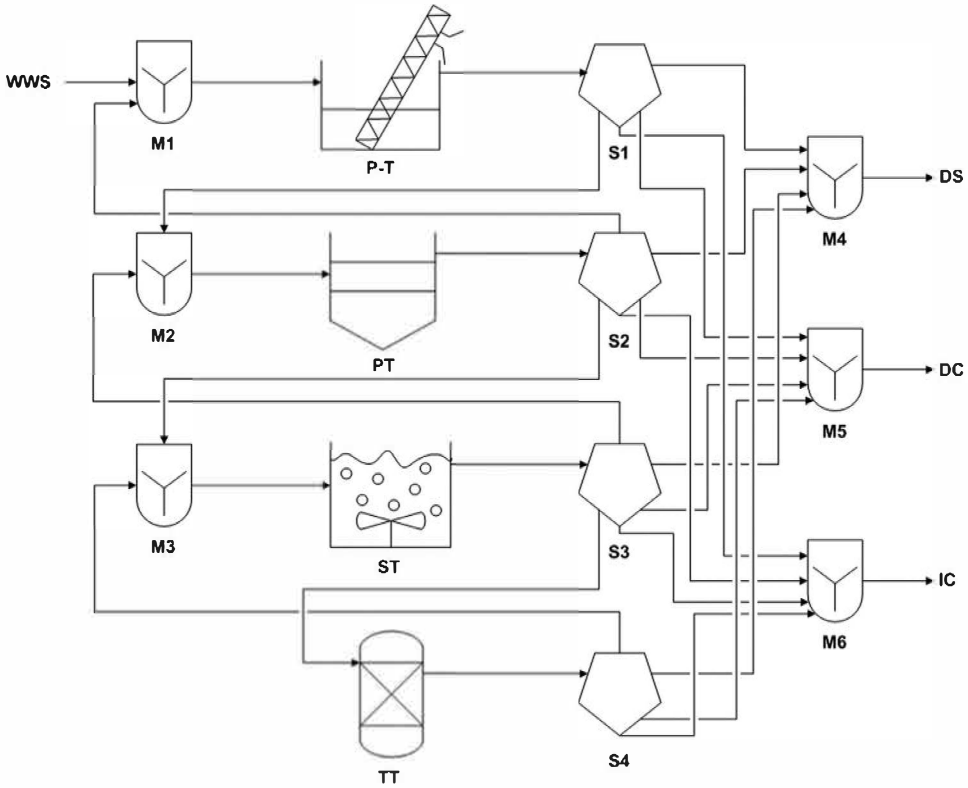

Fig. 3. Superstructure for the WWTP of the case study, which considers one type of discharge (DS), reuse of treated wastewater on public services (DC and IC); and four treatment levels: Pre-treatment (P-T), primary treatment (PT), secondary treatment (ST), and tertiary treatment (TT).

where the concentrations of contaminants in the possible discharge streams ($c_{j,\,ds}$, $c_{j,\,dc}$ and $c_{j,\,ic}$), must fulfill a lower and upper limit ($c^{max}_{j,ds}$, $c^{max}_{j,dc}$, and $c^{max}_{j,ic}$). The logical and structural constraints have a direct impact on the general superstructure for a WWTP. If these constraints are evaluated first, the number of possible configurations (search space) can be reduced. Then, the complexity of the superstructure is reduced, as shown in Fig. 3. This configuration considers one type of discharge (DS), reuse of treated wastewater on public services (DC and IC); and four treatment levels: pretreatment (P-T), primary treatment (PT), secondary treatment (ST), and tertiary treatment (TT).

3.4. Step 4: Model definition

3.4.1. Step 4.a. Benchmarking model retrieval

In this case study, a single constitutive relation is considered, which is the removal efficiency for each pollutant in the different treatment units, considered as a constant value independent of the wastewater flowrate to be treated. In Table 3 the maximum percentage values reported are fixed for the calculation of the amount of pollutant eliminated in the treatment units in Eq. (19):

$$E_{j,h,k} = \frac{pmax_{j,h,k}}{100},\ \forall j \in J, \forall h \in TU,\ \forall\ k \in TL \tag{19}$$

where $E_{j,\,h,\,k}$ is the removal efficiency coefficient of contaminants; and $pmax_{j,\,h,\,k}$ is the maximum percentage of removal reported of pollutant.

3.4.2. Step 4.b. Model development

The proposed process model is based on mass balances for design purposes in terms of the total water flowrates and contaminants concentration, following standard relations. The balances are made around each unit operation of the superstructure, namely, mixers, splitters, and treatment units. A mixer $m \in MU$ considers a set of input streams i specified in the set of indexes M_m and only one output stream o. The mass balance of total water flow and mass balances for each pollutant j in the mixer m are given by Eqs. (20) and (21), respectively:

$$\sum_{i \in M_m} F^i_m = F^o_m,\ \forall\ m \in MU \tag{20}$$

$$\sum_{i \in M_m} F^i_m c^i_{j,m} = F^o_m c^o_{j,m},\ \forall j \in J,\ \forall\ m \in MU \tag{21}$$

where F^i_m is the flowrate of the input stream, F^o_m is the flowrate of the output stream, $c^i_{j,m}$ is the concentration of the contaminant j in the input stream, and $c^o_{j,m}$ is the concentration of the contaminant j in the output stream.

A splitter $s \in SU$ has only one input stream i and a set of output streams o that are specified in the set of indexes S_s. The water flow rate balance for these units is given in Eq. (22). In this case, the concentration of the pollutants is the same for the streams leaving the splitter that for the inlet stream (Eq. (23)):

$$F^i_s = \sum_{o \in S_s} F^o_s,\ \forall\ s \in SU \tag{22}$$

$$c^i_{j,s} = c^o_{j,s},\ \forall j \in J,\ \forall\ s \in SU \tag{23}$$

where F^i_s and $c^i_{j,s}$ are the flowrate and concentrations of the pollutants in the input stream, F^o_s and $c^o_{j,s}$ are the flowrate and the concentration of the pollutant in the output stream.

Each treatment level $k \in TL$ consists of different treatment units ($h \in TU$), specified by the set of indexes, that has one input stream i and one output stream o. Since the concentration of contaminants is low (ppm), it is assumed that the total water flow of the output stream ($F^o_{h,k}$) does not change in the treatment unit (Eq. (24)). The removal efficiency of treatment is $E_{j,\,h,\,k}$ and the binary variable used to choose the treatment is $Y_{h,\,k}$. Thus, the mass balance equation for each contaminant (Eq. (25)), can be expressed as a linear function of the individual contaminant concentration in terms of $E_{j,\,h,\,k}$.

$$F^{i}_{h\,k} = F^{o}_{h.k},\ \ \forall h \in TU,\ \ \forall\ k \in TL \tag{24}$$

$$c^{i}_{j,h,k}\left(1 - E_{j,h,k}\right)Y_{h,k} = c^{o}_{j,h,k},\ \ \forall j \in J, \forall h \in TU,\ \ \forall\ k \in TL \tag{25}$$

3.5. Step 5: Solution strategy

3.5.1. Step 5.a. Mono-objective optimization

The complete optimization model consists of Eqs. (2)–(25) and combines continuous variables with binary variables. The sources of nonlinearities are found in the equations of total cost and the mixer units Eqs. (2) and ((21)). Moreover, Eq. (21) contains bilinear terms, which are a source of non-convexities for the optimization model. Therefore, the proposed optimization model gives rise to a non-convex MINLP problem, which often exhibits local minima and causes convergence difficulties. From the comparative analysis of mono-objective methods, the branch and bound one was selected because it can handle non-convex terms and can find global solutions. Furthermore, to facilitate the decision of whether connections exist or not between treatment units and/or treated wastewater effluents, disjunctions are added to the model:

$$\begin{bmatrix} Y_{dj} \\ F_{ww} \le \max F \end{bmatrix} \vee \begin{bmatrix} Y_{dj} \\ F_{ww} = 0 \end{bmatrix},\ dj \in DJ \tag{26}$$

where Y_{dj} are binary variables, F_{WW} represent the flowrate in the treatment units and/or treated wastewater effluents (continuous variable), and $dj \in DJ$ are the disjunctions. In order to solve this disjunctive programming model, a Big-M relaxation is employed (Eq. (27)), which enables the activation or deactivation of the binary variables (Ramos et al., 2014). M is a large enough coefficient.

$$F_{ww} \le MY_{dj},\ \ dj \in DJ \tag{27}$$

3.5.2. Step 5.b. Multiobjective optimization

For the multiobjective optimization problem, a hybrid method (lexicographic + ε-constraint) is used because it can obtain efficient solutions for problems with non-convex feasible regions containing discrete variables (Mavrotas and Florios, 2013). To apply the proposed hybrid method, the first task is to perform the lexicographic optimization. In the lexicographic method, the objectives are ranked according to the order of importance. The optimization process starts minimizing or maximizing the most important objective and proceeds according to the assigned order of importance of the criteria. On the other hand, for the ε-constraint method, one of the objective functions is optimized while the others are converted into constraints. For this specific case, the total costs are minimized while the environmental aspect (*RE* and *CE*) and the social dimension (*WR*) are taken as restrictions. Considering the maximum and minimum values (payoff table) resulting from the lexicographic optimization, the search of intervals for the constrained objective functions are defined. Hence, by parametrical variation in the right-hand-side of the constrained objective functions the efficient solutions of the problem are obtained. Following this procedure, the Pareto front can be obtained.

3.5.3. Step 5.c. Software and solvers selection

The model coding and solution were performed in GAMS® 24.7, selected since it provides three different MINLP solvers, BONMIN, BARON and COUENNE for handling the formulated problem. The branch-and-bound algorithm of BONMIN is strongly recommended for solving non-convex MINLPs; however, it is a local solver Bonami et al., 2008). BARON is a computational system for solving non-convex optimization problems to global optimality, implementing algorithms of the branch and bound type (Tawarmalani and Sahinidis, 2005). On the other hand, COUENNE aims at finding global optima of non-convex MINLPs. It implements linearization, bound reduction, and branching methods within a branch-and-bound framework (Belotti et al., 2009). The solver BONMIN was discarded because no feasible solutions were obtained for any of the mono-objective optimizations. Regarding global solvers, the best results were obtained considering the solver COUENNE with the Big-M formulation. Therefore, COUENNE was selected as the solver for the WWTP design. In the first instance, the mono-objective optimizations are solved for each of the proposed sustainability criteria (*TC, RE, CE*, and *WR*). The mathematical programming model (Eqs. (2–(25)) was implemented in GAMS® using the solver COUENNE (MINLP) and the Big-M formulation Eqs. (26) and ((27)). The MINLP model involves 712 continuous variables, 237 discrete variables and 693 equations (including constraints). The optimization runs were performed with an Intel (R) Core (TM) i3-6100 U CPU @2.30 GHz processor machine.

3.6. Step 6: Results analysis and selection of the optimal configuration

3.6.1. Step 6.a. Analysis of the pareto front

First, the results concerning the four criteria evaluated separately (mono-objective) are presented in Table 6. For the economic criteria, (*TC*) and energy consumption (*CE*) fewer treatment stages (pre-treatment and primary treatment) are required to meet the goals compared to the others objective functions (*RE* and *WR*), where all treatment levels are considered to find their maxima. The numerical values of the optima for both maximized criteria (*RE* and *WR*) are very similar (Table 6), indicating that these criteria are closely related. Thus, it was decided to omit the environmental criterion (*RE*), because it can be evaluated considering the contaminants concentration limits as an indirect measure of the removal efficiency of contaminants. Consequently, to assess the three dimensions of sustainability, total cost (*TC*), consumed energy (*CE*) and percent of water reused (*WR*) are optimized.

From the mono-objective results, it is observed that *TC, CE*, and *WR* are antagonists, since the numerical values indicate improvement in opposite ways. Then, the tri-objective optimization problem is solved by implementing the hybrid method in GAMS. The results of the lexicographic optimization are presented in Table 7. In the ε-constraint method, one of the objective functions is optimized using the others as constraints. For this specific case, the total costs are minimized while the environmental aspect (*CE*) and the social aspect (*WR*) are taken as restrictions. Considering the maximum and minimum values of the payoff table resulting from lexicographic optimization (Table 7), i.e., *CE* in the range of 2.898–262.346 *GWh/year* and *WR* in the range of 0–100, it is possible to define the search intervals for the ε-constraint method. In Fig. 4, the non-dominated feasible solutions are shown when 21 points are analyzed.

The Pareto fronts (Fig. 4) show monotonically increasing tendencies, except for some points which have a cost decrease while increasing energy consumption (antagonist relation). These points are observed when the percentages of wastewater reused are close to zero (0%–5%). This trend of optimal solutions should be considered when selecting the WWTP design with the best compromise between the evaluated criteria (*TC, CE*, and *WR*), because it could be an error assuming that the increase in total costs, energy consumption and the reuse of treated wastewater is linear and monotonic. Additionally, in order to analyze the antagonistic relationship between *TC, CE* and *WR*, the two-dimensional projections of Fig. 4 are used (Fig. 5–7). The economic and environmental

Table 6
Results of mono-objective optimization.

Criterion	*TC* (*M USD*)	*CE* (*GWh*/*year*)	*RE* (dimensionless)	*WR* (%)
Discharge type	A	A		
Treatment	P-*T*= Screening PT= Flotation	P-*T*= Screening PT=Filtration	P-*T*= Screening PT= Filtration ST= Anaerobic processes TT= Membranes	P-*T*= Grit separator PT= Primary sedimentation ST= Anaerobic processes TT= Membranes
Flow treated (m^3/d)	P-*T* = 6480,000 PT=1682,783 DS=6480,000	P-*T* = 6480,000 PT= 1998,304 DS= 6480,000	P-*T* = 6480,000 PT= 6480,000 ST= 6480,000 TT= 6480,000 DC=6480,000	P-*T* = 6480,000 PT= 6480,000 ST= 6480,000 TT= 6480,000 DC=6480,000
TC (*M USD*)	**13.411**	37.103	731.969	751.077
CE (*GWh*/*year*)	19.136	**2.8977**	1410.369	1423.141
WR (%)	0	0	100	**100**
RE (dimensionless)	0.495	0.918	**4**	4
Concentration in the discharge (kg/m^3)	BOD_5= 0.198 TSS= 0.20 TN= 0.026 TP= 0.01	BOD_5= 0.186 TSS= 0.20 TN= 0.02 TP= 0.008	BOD_5= 0 TSS= 0 TN= 0 TP= 0	BOD_5= 0 TSS= 0 TN= 0 TP= 0
Concentration in DC (kg/m^3)	BOD_5= 0 TSS= 0 TN= 0 TP= 0	BOD_5= 0 TSS= 0 TN= 0 TP= 0	BOD_5= 0 TSS= 0 TN= 0 TP= 0	BOD_5= 0 TSS= 0 TN= 0 TP= 0
Concentration in IC (kg/m^3)	BOD_5= 0 TSS= 0 TN= 0 TP= 0	BOD_5= 0 TSS= 0 TN= 0 TP= 0	BOD_5= 0 TSS= 0 TN= 0 TP= 0	BOD_5= 0 TSS= 0 TN= 0 TP= 0
Resolution time (*s*)	404.4	816.1	510.9	794.6

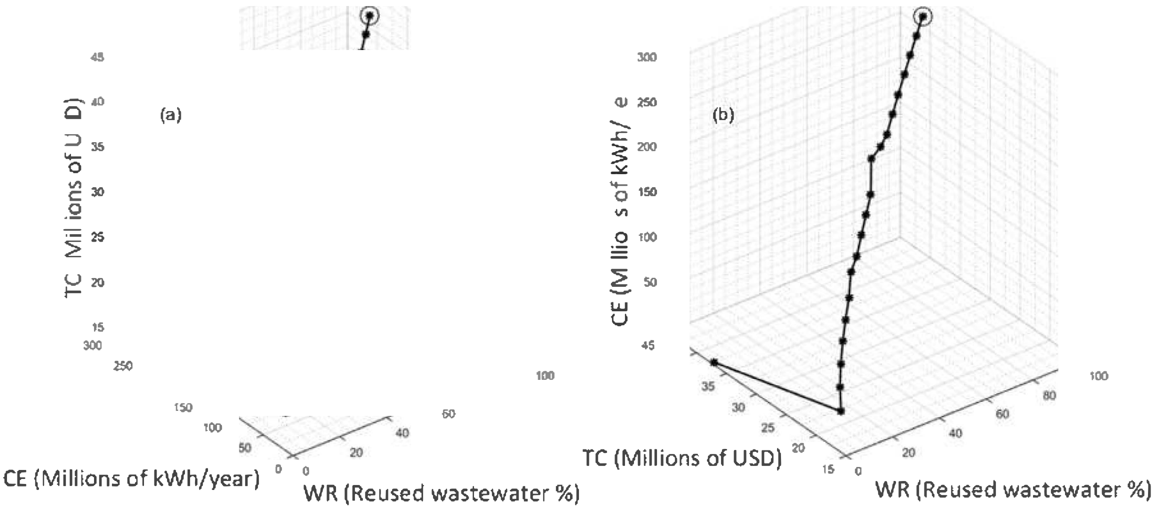

Fig. 4. (a) 3D-Pareto front for *WR*, *CE* and *TC* for optimal WWTP design and (b) 3D-Pareto front for *WR*, *TC* and *CE* for optimal WWTP design.

Table 7
Results obtained for lexicographic optimization.

	Minimize *TC*	Minimize *CE*	Maximize *WR*
TC (*M USD*)	**13.411**	37.103	41.303
CE (*GWh*/*year*)	19.136	**2.898**	262.346
WR (%)	0	0	**100**

aspects have a direct relationship, except for some points, which have a cost increase while decreasing energy consumption (antagonist relation). Regarding the social criterion. this has an inverse relationship, that is, to increase the percentage of reclaimed water, the costs and energy consumption also must increase. Even though the energy consumption does not present a generally antagonistic relationship with the total costs, it is a decisive criterion for obtaining the optimal configurations of the WWTP represented on the Pareto front. The above can be corroborated since the dominated solutions did not comply with the energy consumption restrictions. Fig. 8

3.6.2. Step 6.b. Multiple criteria decision making

So far, the question of how to choose the best trade-off solution among those of the Pareto fronts remains. For the case study, the three criteria *TC*, *CE* and *WR* should be considered together, and the decision cannot be done if one of these objectives is excluded. M-TOPSIS method is implemented in MATLAB® R2015a. The weights are considered to have the same value for all criteria (equally important).

In Table 8, the resulting order of balanced criteria for the WWTP is presented. Then, the best choice for the treatment plant has the following numerical values $CT = 41.303$ M USD, $CE = 262.346$ $GWh/year$, and $WR = 100$, this solution is highlighted

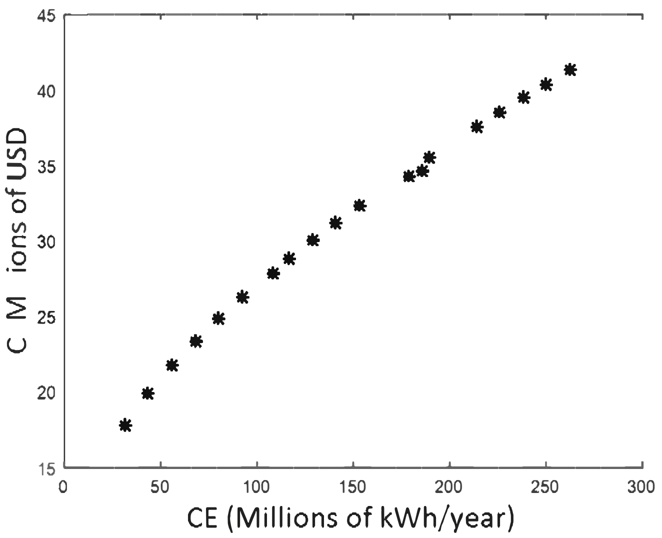

Fig. 5. Two-dimensional projection of the Pareto Front for *TC* and *CE* criteria.

Table 8
M-TOPSIS analysis results.

M-TOPSIS ranking	Total Cost (*M USD*)	Consumed Energy (*GWh/year*)	Water Reused (dimensionless)
1	41.303	262.346	100
2	30.043	128.581	45
3	31.21	140.741	50
4	28.832	116.42	40
5	32.344	153.394	55
6	17.77	31.297	5
7	27.879	108.435	35
8	26.248	92.099	30
9	40.387	250.186	95
10	37.103	2.898	0
11	24.851	79.94	25
12	19.93	43.457	10
13	35.533	189.383	70
14	23.359	67.778	20
15	34.604	185.39	65
16	21.74	55.618	15
17	34.242	178.682	60
18	39.455	238.025	90
19	36.546	201.544	75
20	37.536	213.704	80
21	38.505	225.865	85

within a circle in Fig. 4. The optimal configuration for this WWTP is presented in Fig. 6. The considered techniques (screening, flotation, and anaerobic processes) have a common characteristic, all are capable of selectively remove BOD_5 and TSS, which is one of the determining factors for the selection, since these contaminants are the ones of greater proportion. In addition, the anaerobic process of the secondary treatment stage is mainly applied for the treatment of sludge, however, in this WWTP is presented as an appropriate alternative for the treatment of wastewater. Regarding the type of configuration, a decentralized arrangement is obtained, in which the effluent from the primary treatment (flotation) is divided to avoid unnecessary treatment of the stream.

The selected WWTP is an extreme point in the Pareto front that satisfied the direct relationship between total costs and consumed energy. Even though the Pareto front presents a general trend of growth for all objectives, the M-TOPSIS ranking does not follow a uniform selection trend. The above is verified by analyzing the data in Table 7, for example, option 9 of the ranking considers 95% of water reused and the option that follows (option 10) considers 0% of water reused. On the other hand, from a design perspective,

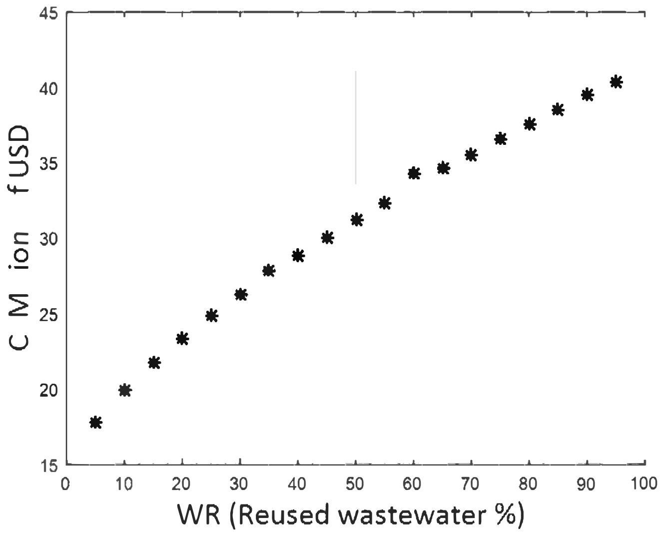

Fig. 6. Two-dimensional projection of the Pareto Front for *TC* and *WR* criteria.

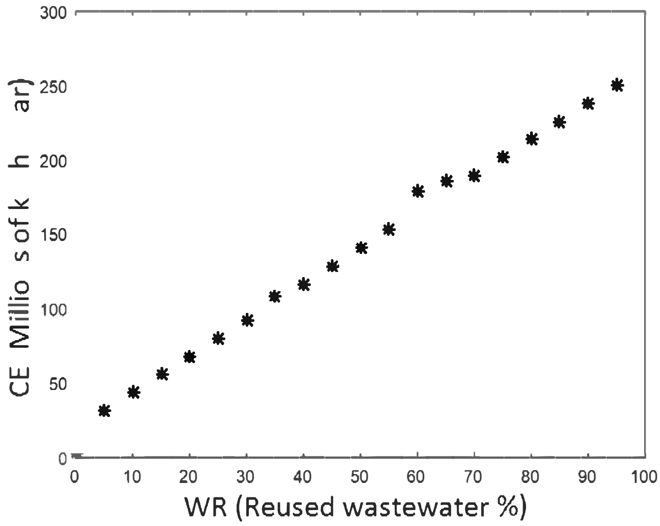

Fig. 7. Two-dimensional projection of the Pareto Front for *CE* and *WR* criteria.

not all treatment combinations involve energy consumption in the same proportion while the total cost is highlighted, that is, there are treatment techniques that consume low energy but are expensive, for example, filtration. Thus, the amount of energy used in a WWTP should not be discarded a priori as a decision criterion when some cost function is evaluated. This suggests that even in particular instance, the economic criteria and the consumed energy are antagonistic. Therefore, a configuration for which the direct relationship is not fulfilled exists. In addition, it is necessary to integrate other types of energy use in the design of a WWTP to make evident the difference between these criteria (like chemical and thermal energy).

Comparing the optimal WWTP design obtained in this work with the current and actual WWTP, this one removes contaminants such as fats, oils, and pathogens, but maintains a good part of the nutrients. Its treatment techniques are screening, grit separator, primary sedimentation, aerobic process, and chlorine disinfection (CONAGUA, 2018); with $TC = 623.06\ M\ USD$, $CE = 328.763\ GWh/year$, and $WR = 100\ \%$. Our proposed optimal WWTP has substantial design differences with the actual one, since this operates through an activated sludge scheme, and the optimal one considers an anaerobic process for secondary treatment and a

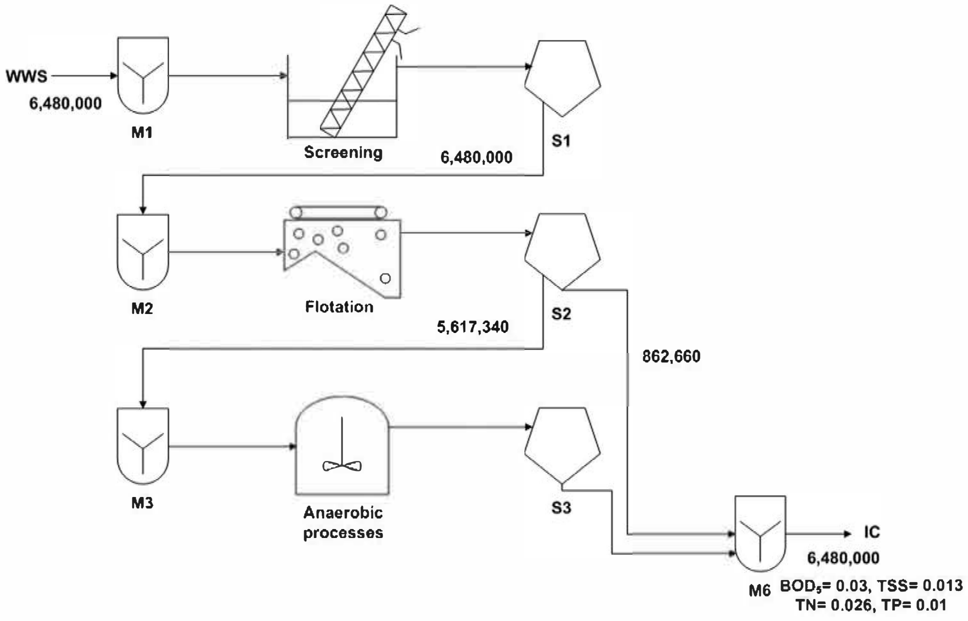

Fig. 8. The best trade-off configuration for the WWTP according to the M-TOPSIS analysis. The flowrates have units of m^3/d and the concentration of the contaminants have units of kg/m^3.

flotation process for primary treatment. Nevertheless, both designs have in common that the amount of nutrients is enough to be used for irrigation purposes, the best design, applying the multi-optimization framework for sustainable WWTPs, improved the total cost and the energy consumption: $TC = 41.303\ M\ USD$, $CE = 262.346\ GWh/year$.

4. Conclusions

An integrated methodology that combines conceptual and mathematical programming approaches for designing sustainable WWTPs has been proposed and applied to a municipal wastewater case study from Mexico City. This six-step procedure enables the identification, comparison, and screening of WWTP options, through bottlenecks identification, constraints, and objective functions evaluation. Four metrics were assessed (total cost -TC-, removal efficiency -RE-, consumed energy -CE-, and wastewater reused -WR-), to address sustainable development. Nevertheless, only three criteria showed antagonistic relations (removal efficiency was not retained). The implementation of a hybrid optimization method (lexicographic + ε-constraint) provided a set of different optimal design options in the form of a Pareto front, when the three sustainability criteria were considered simultaneously. Finally, to balance the trade-off between economic, environmental and social aspects, a MCDM analysis was implemented by M-TOPSIS and the best trade-off solution was identified. Multiobjective optimization results confirmed the importance of studying the three aspects of sustainability at the same time (reduction of 93.4% in TC, 20.2% in CE). These results can serve as guidance for decision makers (e.g. politicians) to define new laws and to understand the implication of the forthcoming legislation in the sustainable performances of the companies and cities.

One of the main drawbacks of the implementation of the developed framework is the data availability and quality. The use and/or development of a knowledge-based system, as a systematic tool based on technical, economic, environmental and social criteria, is recommended. On the other hand, this work focuses only on the treatment of the liquid phase of wastewater while the treatment of sludge obtained from wastewater plays an important role. The inclusion of the sludge treatment stage in the superstructure of the treatment network is considered as future work.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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Supplementary materials

Supplementary material associated with this article can be found, in the online version, at doi:10.1016/j.compchemeng.2020.106850.

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