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# Targeting economic and environmental benefits associated with the integration of regeneration units in water systems

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ABSTRACT

Water treatment is traditionally seen as an "end-of-pipe" solution to deal with contaminated water satisfying discharge regulations at a minimum expense. However, the reuse of treated water as regenerated water is a promising strategy to counteract water scarcity. This approach to transform waste into resources is motivated by the circular economy paradigm. This study presents a mathematical programming approach to target both the environmental and economic benefits of water systems by introducing additional regeneration units to close the loop. In addition to water users and authorities, the approach also considers operators and dealers, which are revealed as key stakeholders. Hence, the feasible region of the regeneration units design specifications is determined and visualized through a multi-objective optimization approach targeting the systems operating cost and freshwater consumption. Its application is demonstrated on a benchmark case study from the literature, revealing a potential economic benefit of 37.5% and a freshwater reduction of 80.9% over the case without regeneration units. Furthermore, we show that a cooperative exchange strategy leads to higher benefits compared to the solutions presented in the literature. Finally, we demonstrate how the barrier plots introduced in this work can be used by different stakeholders in the water market to support their decision-making.

## 1. Introduction

Freshwater resources are increasingly stressed and polluted due to the improvement of living standards, population growth (Shannon et al., 2008) and climate change (Schewe et al., 2014). The Sustainable Development Goals report (United Nations, 2020) reveals that global progress towards the “availability and sustainable management of water and sanitation for all” (Goal 6) at its current pace will not meet the target by 2030. This would lead to an estimated displacement of 700 million people due to water scarcity. The main inhibiting aspect is a funding gap to realize the necessary change.

Circular Economy (CE) is a concept and potential solution that has gained traction with the increasing awareness of sustainability issues starting in the 1970s (Ellen MacArthur Foundation, 2013). It is an alternative to the “take-make-waste” linear economy model and dictates that circular material loops have the potential of leading to environmental but also economically beneficial situations. Applying some concepts of circular economy, such as material reuse and upcycling, to the design of water systems could help render the funding gap issue null.

Freshwater consumption can be reduced by replacing freshwater in processes that have low water quality demand with wastewater of low contamination from another process. If the quality of wastewater is too low for direct reuse, a treatment process can reduce the contamination level, thereby enabling recycling of such regenerated water. Treatment processes can be classified in primary (e.g. clarification), secondary (e.g. membrane bioreactors) and tertiary (e.g. advanced oxidation processes). Henceforth we refer to any system accepting wastewater and discharging regenerated water, consisting of one or more treatment processes, as Regeneration Unit (RU). In order to comply with environmental regulations, traditionally “end-of-pipe” solutions are considered for disposing contaminated water. However, under the right conditions, RUs can act as CE enablers by feeding back the regenerated water to the supply chain, helping to reduce freshwater consumption in markets suffering from water scarcity and possibly generating payoff.

A variety of water integration solutions have been demonstrated on all scales: individual industries (Karuppiah and Grossmann, 2006), (eco-) industrial parks (Ramos et al., 2016), municipalities (Chhipi-Shrestha et al., 2019), and even on the scale of entire countries (Saidan

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et al., 2020). For an overview of open challenges and opportunities of establishing a circular economy in the water sector the reader is referred to the review by Guerra-Rodríguez et al. (2020). They conclude that besides safety, regulatory and cultural issues, the financial outlay is a main challenge. Sgroi, Vagliasindi and Roccaro (2018) discuss the feasibility and sustainability of CE solutions in water reuse. They arrive to the same conclusion and highlight the need for a holistic approach considering political, decisional, social, economic, technological and environmental factors.

The optimization of water systems for economic and environmental objectives has been extensively studied. Ahmetovic, Grossmann, Kravanja and Ibric (2017) provide an overview of the strategies that have been developed and applied to the process industry. Pinch-based strategies are one of the main approaches to solve water exchange problems, allowing graphical interpretation and giving insight into the water systems interactions. Selected recent advances in Pinch-based methodologies are related to automation and sensitivity analysis (Parand et al., 2016) and multi-contaminant treatment (Chin et al., 2021). The other main branch of water system optimization relies on superstructure generation and mathematical programming. Early works proposed efficient methodologies to solve large scale water systems for single objectives (Karuppiah and Grossmann, 2006), while recent advances rely on heat-integrated water networks that capture also the energy targets of water systems. These are solved using multi-stage sequential (Ibrić et al., 2021) or simultaneous solution strategies (Kamat et al., 2019). Lee, Tsai and Foo (2020) recently contributed a generic mathematical model for the retrofitting of existing water networks and provided trade-off solutions for freshwater consumption, retrofit cost and network complexity.

However, these studies are oriented and limited to here-and-now situations with a single fixed or a small set of RUs. In order to debottleneck the progression towards targeted goals such as the Sustainable Development Goals it is important to answer the reverse question: what are the necessary conditions of a regeneration unit to reach a desired situation? To that end, this contribution proposes a novel approach and a holistic methodology based on mathematical programming to reveal the technological (treatment efficiency) and economical (treatment cost) conditions that a RU must fulfill in order to ensure economic and environmental benefits in a selected market.

We focus on demonstrating the capabilities of the methodology to be easily applied to different markets and conditions, as well as its usefulness as a decision support tool for the three main stakeholders in the water supply chain:

(1) **Water users** (industry, agriculture, households) that use water with the objective to buy the least necessary amount at the lowest possible cost.
(2) **Authorities** with the environmental objective to reduce freshwater scarcity through reduced consumption.
(3) **Operators** of centralized regeneration units that aim to improve their economic performance through reduced operational cost or payoff from selling regenerated water to users at higher cost.

Although the latter is not usually regarded as a main stakeholder in optimization problems, it is a key piece in the expansion of the limits of water upcycling towards circular water systems.

## 2. Water regeneration units as CE enabler

The advantages of water regeneration have been studied and applied to water systems for over four decades but, with the recent interest in CE, research has taken a new turn through water integration and exchange. A remarkable example of this can be found in the application to eco-industrial parks (EIPs). Lovelady and El-Halwagi (2009) presented a mathematical programming formulation for source regeneration-sink matching in water systems of EIPs minimizing an economic objective function of the water users. Boix, Montastruc, Pibouleau, Azzaro-Pantel and Domenech (2011) first acknowledged the potential of further decreasing the freshwater consumption beyond the economically optimal solution by formulating a multi-objective optimization problem, considering the trade-off between freshwater consumption and necessary treatment cost. They consider multi-contaminant systems and propose a strategy for choosing an optimal solution among the Pareto optimal ones. Ramos, Boix, Montastruc and Domenech (2014) applied Goal Programming to the same type of problems to avoid the necessity to determine the complete Pareto front. Later, the same authors applied a multi-leader-follower formulation stemming from Game Theory to find balanced solutions taking into account the hierarchy of different stakeholder in an EIP (Ramos et al., 2016). In a recent work by Salas et al. (2020) the aspect of non-cooperative behavior and limited shared information among water users in a water market was further developed by formulating a blind-input single-leader multi-follower game and transforming it into a mathematical program.

In municipal applications the use of regenerated water has been practiced for a long time in irrigation of agricultural land and green areas. In fact, this practice is intuitive and reasonable if the RU can ensure that the remaining contamination poses negligible health related risk. The potential economic benefit can be huge and Chen et al. (2013) conclude that it should be encouraged. Going beyond the studies that demonstrate payoff generation in inter-plant and EIP scenarios, Somoza-Tornos et al. (2019) presented a study showing that municipal Wastewater Treatment Plants (WWTP) can generate payoff by identifying customers and supplying them with regenerated water. In contrast to other studies that neglect the point of view of the RUs, the approach taken by Somoza-Tornos et al. (2019) focuses on the WWTP point of view.

It is worth noting that some RUs can also promote CE by various types of waste and sludge valorization techniques as demonstrated for example in Trinh et al. (2021) for the recovery of copper from sludge obtained from WWTPs. Gherghel, Teodosiu and De Gisi (2019) give an overview of various techniques for recovery of other heavy metals, nutrients, construction materials, bio-plastics, proteins and enzymes.

Those practices are still new but could potentially further contribute to the circularity of the water sector and the economic independence of RUs in a circular water market. There is a significant global movement towards valorizing sludge and wastewater as can be seen for instance in the position paper by Water Europe (Water Europe, 2021), highlighting the joined efforts of over 200 members from academia, industry and other water users, providers and authorities in the European Union. For instance, Smol et al. (2020) propose a circular economy model framework in the European water and wastewater sector. Reclamation, reuse, recycle and recovery are four of the six key actions of the proposed framework and their main novelty is the assessment of organizational and societal changes. Nika, Vasilaki, Expósito and Katsou (2020) present another circularity assessment framework for complex water systems. They developed an indicator database including existing and newly proposed indicators to assess multi-sectoral systems circularity.

Side revenues, environmental payoff from energy and raw material reclamation processes and other legal and/or multi-sectoral considerations are not part of this work but mapping their barriers could follow the same procedure as presented herein. Fig. 1 depicts the circularity in the water market covering water circularity on one hand and contaminant circularity on the other hand. This first work focuses on the water circularity part while considering the scalability and extensibility of the general framework that would integrate the complete circularity of the water supply chain in future developments.

## 3. Problem statement

Benefits must be assessed quantitatively over a reference case. To that end, we define three different collaboration scenarios of increasing water exchange potential as depicted in the superstructures in Fig. 2. An

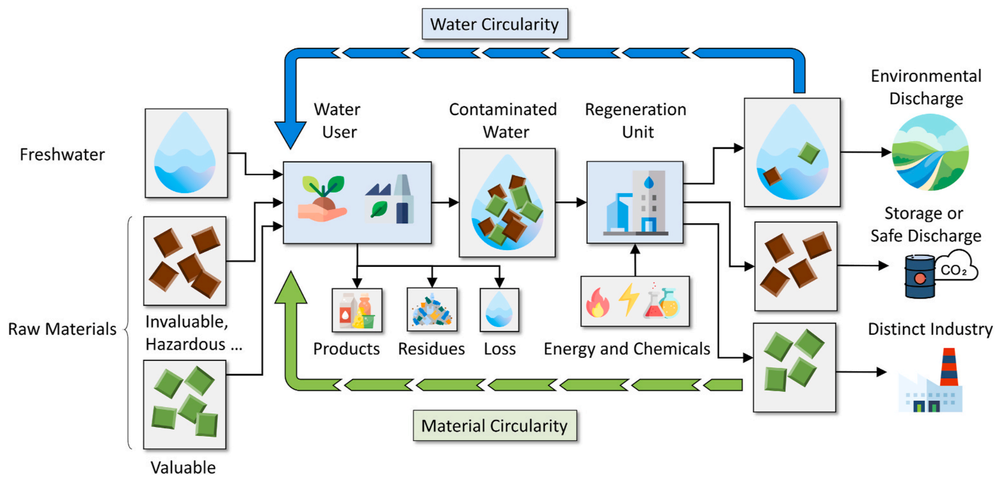


**Fig. 1.** Circularity in the water supply chain.

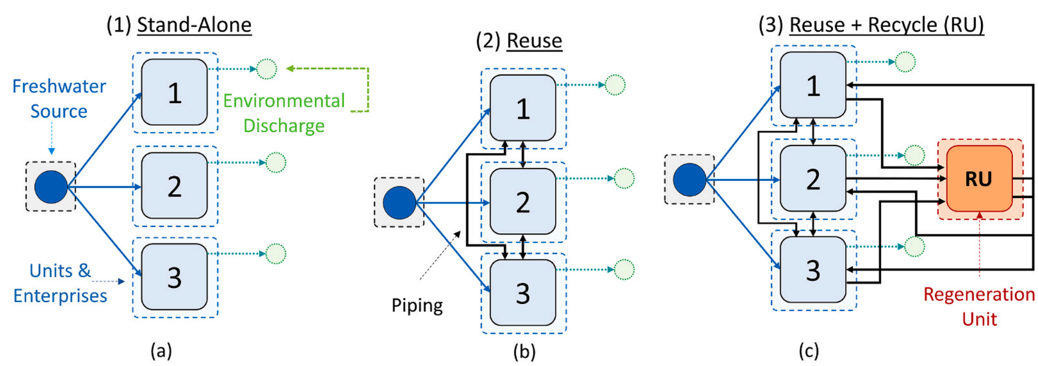


**Fig. 2.** Conceptual water exchange scenarios between water using units and enterprises.

enterprise is considered to be a group of water using units with a shared economic objective (e.g. a chemical company). RUs are treated as a special kind of enterprise where the economic objective is captured in the selling price of regenerated water. In the standalone scenario (Fig. 2 (a)) water exchange between enterprises does not take place. Within an enterprise, units are allowed to exchange water but the remaining water demands must be satisfied by freshwater. The freshwater consumption is the highest in this case. The second scenario is the direct reuse case (Fig. 2 (b)) in which water exchange between enterprises can take place through piping but in the absence of regeneration units. In this case, the reduction of freshwater consumption is limited only to applications that can use already used water directly (e.g. refrigeration water used for cleaning). The third scenario is the regeneration and recycle case (Fig. 2 (c)) and it comprises a regeneration unit to overcome the limitation by treating wastewater and further reduce freshwater consumption in the system.

The general problem can be posed as follows: Determine the limiting technological and economical barriers for RUs to profitably enter a market. To that end, solve a set of water exchange network design problems, maximizing the achievable economic and environmental benefit by introducing a set of RUs to the market. Given:

- A set of enterprises E comprising water using units.
- The associated subsets of water using units $U_e$ with their respective contaminant loads, inlet and outlet contaminant concentration limits and flow constraints.
- A set of RUs $U_{RU}$ as a special variant of water using units with fixed outlet contaminant concentrations or removal ratios.
- A set of contaminants J.
- A set of freshwater sources F with associated quality and cost.
- Environmental discharge limits and cost.
- Other technical and economic data (e.g. piping cost, distance between units).

Prior to solving the regeneration and recycle case with the RUs that are to be integrated to the system, the standalone and reuse cases must be solved as references for the targeting task. Here, we opt for determining the networks with a minimum cost in both cases but other criteria such as the freshwater consumption, network complexity or contaminant discharge to the environment could be chosen.

## 4. Methodology

### *4.1. Base model summary*

The underlying base model comprises standard water and contaminant balances that are listed in Appendix A. The nomenclature is illustrated in Fig. 3.

In this work, we introduce water regeneration units to model the

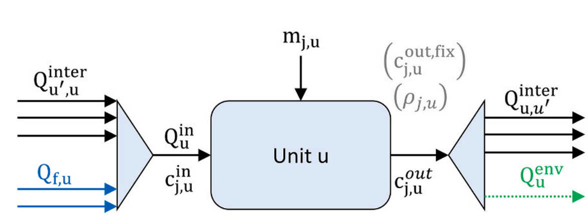


**Fig. 3.** Material balance for a general water using unit.

reduction of the concentration of contaminants. A comparison between the different modeling assumptions about the operation of the RU is made. RUs can be modeled as fixed outlet concentration units that guarantee a maximum effluent contamination of $c_{j,u}^{out,fix}$. In this case the outlet contaminant balance takes the form of Equation (1).

$$c_{j,u}^{out} = c_{j,u}^{out,fix} \ \forall u \in U_{RU} \ \forall j \in J \tag{1}$$

Alternatively, the RU may be modeled as fixed removal ratio unit which reduces the incoming contaminant concentration by a fixed ratio $\rho_{j,u}$ as indicated in Equation (2). The implications of these two modeling alternatives are discussed later on.

$$c_{j,u}^{out} = c_{j,u}^{in} \cdot \left(1 - \rho_{j,u}\right) \ \forall u \in U_{RU} \ \forall j \in J \tag{2}$$

Inlet and outlet contamination levels are bounded by $c_{j,u}^{in,max}$ and $c_{j,u}^{out,max}$ in Equations (3) and (4).

$$c_{j,u}^{in} \leq c_{j,u}^{in,\max} \quad \forall u \in U_{RU}, U_e \ \forall j \in J \tag{3}$$

$$c_{j,u}^{out} \leq c_{j,u}^{out,\max} \quad \forall u \in U_{RU}, U_e \quad \forall j \in J \tag{4}$$

### 4.2. Objectives

The set of economic objectives $OF1_e$ denotes the set of operational costs of each enterprise $e$. It comprises the freshwater, discharge, interchange and regeneration cost.

$$OF1_e = \sum_{u \in U_e} \sum_{f \in F} Q_{f,u} \cdot C_f + \sum_{u \in U_e} Q_u^{env} \cdot C^{env} + \frac{C^{pipe}}{2} \cdot \sum_{u \in U_e} \sum_{u' \in U_e} \left( Q_{u',u}^{\text{inter}} + Q_{u,u'}^{\text{inter}} \right) + \sum_{u \in U_e} \sum_{u' \in U_{RU}} C_{u'}^{reg} \cdot \left( Q_{u',u}^{\text{inter}} \right)^{\psi} \qquad \forall e \in E \tag{OF1}$$

Connected units equally share piping cost. This work considers a single RU with regeneration cost $C_{u'}^{reg} = \gamma$. The power $\psi < 1$ in the regenerated water cost term accounts for economy of scale, meaning that higher effluent flowrates can be treated at lower cost.

It should be noted that the capital cost of constructing a RU plays a significant role and influences the barriers to its integration. For the sake of comparability with the referred literature case-study Ramos et al. (2016) we opted for using the same economic objective function, which does not include the capital cost. However, its extension and inclusion would be straightforward.

The global environmental objective chosen is the minimization of freshwater consumption as a main countermeasure against water scarcity.

$$OF2 = \sum_{u \in U_e} \sum_{f \in F} Q_{f,u} \tag{OF2}$$

The methodology is flexible enough to handle alternative economic and environmental objectives. Despite not being considered in this work, social objectives such as the amount of jobs related to the water system or human toxicity potential from contaminant discharge might be taken into account. The selection of relevant objectives depends on the decision-makers' preference.

#### 4.2.1. Targeting problem

The targeting problem comprises the determination of the optimal network configurations for reaching a specified economic and environmental benefit over a non-regeneration reference case. The complete targeting problem is decomposed into a series of subproblems. The solution strategy involves the solution of the standalone and reuse cases that are defined by the mathematical programs OP1 and OP2 respectively. Once the reference values for the targeting problem are obtained, the economic and environmental targeting problems are solved, as defined in OP3.

The standalone case departs from the assumption that the enterprises in the market do not initially engage in water exchange. In a first step, the operating cost of each enterprise is minimized, allowing water exchange within the enterprise without constraints on the freshwater consumption. The standalone case is defined in OP1 and is solved for each enterprise where the structure defining parameter $x$ is chosen to prohibit exchanges between distinct enterprises.

$$\min_{Q} OF1_e^{(1)} \ \ \forall e \in E \tag{OP1}$$

$$s.t. \ (A1) - (A10) \ \wedge (1) - (4)$$

OP2 defines the reuse case. Constraints on the operating cost of each enterprise $OF1_e^{(2)}$ and the freshwater consumption $OF2^{(2)}$ are added. Water exchange between enterprises is allowed by changing the structure governing parameters $x$.

$$\min_{Q} \sum_{e \in E} OF1_e^{(2)} \tag{OP2}$$

$$s.t. \ (A1) - (A10) \ \wedge (1) - (4)$$

$$OF1_e^{(2)} \leq OF1_e^{(1)} \ \forall e \in E$$

$$OF2^{(2)} \leq OF2^{(1)}$$

Finally, taking the minimal operational cost from the direct reuse case as new reference, the methodology allows for targeting economic and environmental benefits by adding constraints that limit the economic and environmental objectives by a portion α and β, respectively:

$$\sum_{e \in E} OF1_e^{(3)} \leq (1 - \alpha) \cdot \sum_{e \in E} OF1_e^{(2)} \tag{5}$$

$$OF2^{(3)} \leq (1 - \beta) \cdot OF2^{(2)} \tag{6}$$

The resulting optimization problem OP3 is given as follows:

$$\min_{Q} - \alpha \ \vee \ -\beta \tag{OP3}$$

$$s.t. \ (A1) - (A10) \ \wedge (1) - (4)$$

$$OF1_e^{(3)} \leq OF1_e^{(1)} \ \forall e \in E$$

OP3 is a Mixed-Integer Nonlinear Problem (MINLP). It must be solved for a range of RU specifications ($c_{j,u}^{out,fix}$ and $\gamma$) in order to obtain the response surfaces to the economic ($\alpha > 0, \ \beta = 0$) and environmental ($\alpha = 0, \ \beta > 0$) targeting problems. We introduce the barrier plots for the integration of RUs into systems of water users which stands as a novel contribution for decision-making support (see Fig. 4).

The design of experiments to determine the response surface is a trade-off between the desired accuracy and the computational expense. First, a solver must be chosen and tuned to calculate the data points. Conservative approximations to the surface can be found faster using a smaller optimality tolerance. A variety of strategies can be applied to

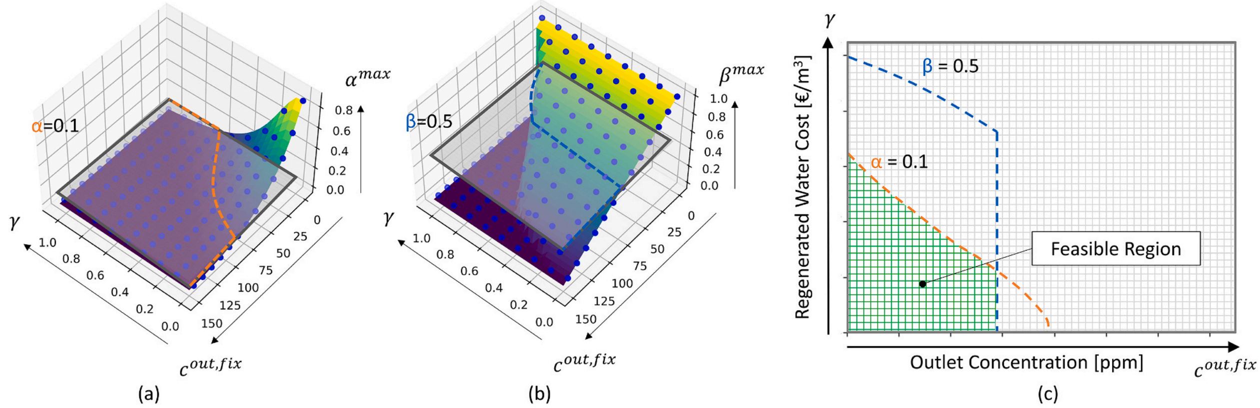


**Fig. 4.** Economic (a) and environmental (b) targeting response surfaces. Blue dots mark the solved cases. (c) Construction of the feasible RU design region for targeting α = 0.1 and γ = 0.5.

determine the set of $c_{j,u}^{out,fix}$ and $\gamma$. For problems of low complexity, a full-factorial design can be applied.

Once the pure economic and environmental targeting problems are solved (Fig. 4 (a) and (b)), any mixed targeting problem ($\alpha > 0,\ \beta > 0$) solution can be derived through superposition. Fig. 4 (c) shows how the two limiting areas from the economic targeting and environmental targeting are combined to yield the feasible region of the mixed targeting problem. When targeting a specific combination of $\alpha$ and $\beta$ the contour plot in the desired $\alpha$ and $\beta$ planes can be used to draw the limiting conditions of a RU to reach that desired target (Fig. 4 (c)). For targets where $\alpha > \beta$ the barrier will follow the contour from the economic targeting problem. This is because for a given $c_{j,u}^{out,fix}$ and $\gamma$ it can be shown that the solution to the economic targeting problem is smaller than the environmental problem ($\alpha^{max} < \beta^{max}$). For a larger $\beta$ the constraint (6) becomes active. The feasible design region for the RU is then the area under the superposition of the economic and environmental barrier as depicted in Fig. 4 (c).

Examples for the possible ways of interpreting the data from different points of view are as follows:

- Enterprises can come together to reveal unexploited cooperation potential. If not governed by an authority, the analysis can be restricted to the economic targeting problem ($\alpha > 0,\ \beta = 0$).
- Local authorities can devise strategies to reduce the environmental impact in their region while also assuring a minimum economic incentive to the enterprises ($\alpha \geq 0,\ \beta \gg 0$).

**Table 1**
Input data adapted from Ramos et al. (2016).

| Enterprise | Unit | $C^{in,max}$ | $C^{out,max}$ | $m$ | $Q_u^{max}$ |
|---|---|---|---|---|---|
| - | - | ppm | ppm | $gh^{-1}$ | $m^3h^{-1}$ |
| *e1* | u11 | 0 | 100 | 2,000 | 100 |
| | u12 | 50 | 80 | 2,000 | 125 |
| | u13 | 50 | 100 | 5,000 | 250 |
| | u14 | 80 | 800 | 30,000 | 190 |
| | u15 | 400 | 800 | 4,000 | 25 |
| *e2* | u21 | 0 | 100 | 2,000 | 100 |
| | u22 | 50 | 80 | 2,000 | 125 |
| | u23 | 80 | 400 | 5,000 | 65 |
| | u24 | 100 | 800 | 30,000 | 190 |
| | u25 | 400 | 1,000 | 4,000 | 20 |
| *e3* | u31 | 0 | 100 | 2,000 | 100 |
| | u32 | 25 | 50 | 2,000 | 200 |
| | u33 | 25 | 125 | 5,000 | 200 |
| | u34 | 50 | 800 | 30,000 | 190 |
| | u35 | 100 | 150 | 15,000 | 500 |

$Q_u^{min} = 2m^3h^{-1}$

- RU operators may perform such analysis on several markets to reveal business opportunities.

It must be acknowledged that the applicability and performance of this methodology strongly depends on the availability and reliability of the market data, i.e. demands, constraints and costs.

## 5. Case study

We employ input data in the scale of an EIP adapted from Ramos et al. (2016) in Table 1 with the intention to characterize the market in terms of economic and environmental saving potential. By doing so, we further analyze the optimality of the solutions provided in the literature as well as discuss the RU design specifications. We have chosen this hypothetical EIP data as a case study because it is a widely studied benchmark system (Boix et al., 2012; Chew et al., 2009; Olesen and Polley, 1996). A direct comparison of the solutions resulting from our methodology to the solutions provided in the literature will reveal the implications of cooperative (here) and non-cooperative (literature) strategies in water systems, an insight that will be useful for decision-making and strategizing.

Limiting inlet flowrates $Q_u^{max}$ are added to prevent unreasonably high dilution rates for low performing regeneration units. For the regeneration unit this value is set to 1,200$m^3h^{-1}$ (50% of maximum system load). Furthermore, the nonlinear power term $(Q_{u',u}^{inter})^{\psi}$ in the economic objective function has been replaced with a piecewise linearized function as described in Appendix B.

Cost parameters are summarized in Table 2. It must be noted that all parameters are chosen by the authors to lead to a clear economic and environmental benefit when integrating RUs. However, if the analysis reveals that no or very small benefits can be achieved, this tells the stakeholder that other strategies must be used to reach the targets.

## 6. Results and discussion

We focus the comparison of the results to the original formulation and solutions by Ramos et al. (2016). They solve the standalone case for each enterprise (Table 3) as well as three distinct problem formulations for the reuse (Table 3) and regeneration and recycle cases (Table 4).

**Table 2**
Cost parameters.

| | |
|---|---|
| Environmental Discharge ($C^{env}$) | 0.22 €/$m^3$ |
| Freshwater ($C_f$) | 0.13 €/$m^3$ |
| Piping ($C^{pipe}$) | 0.02 €/$m^3$ |

**Table 3**
Standalone and reuse solutions.

| | Operating Cost (OF1) [$10^6$ €/year] | | | | Freshwater Consumption [$m^3$/h] | | | |
|---|---|---|---|---|---|---|---|---|
| | e1 | e2 | e3 | Total | e1 | e2 | e3 | Total |
| *Standalone*[(a)] | 0.28 | 0.16 | 0.54 | 0.98 | 98.33 | 54.64 | 186.67 | 339.64 |
| *MOO-GP*[(b)] | 0.20 | 0.13 | 0.61 | 0.94 | 88.33 | 20.00 | 206.02 | 314.36 |
| *MLSFG*[(b)] | 0.27 | 0.15 | 0.54 | 0.95 | 146.67 | 33.62 | 134.06 | 314.35 |
| *SLMFG*[(b)] | 0.26 | 0.16 | 0.54 | 0.95 | 136.59 | 39.34 | 138.42 | 314.35 |
| *OP2*[(c)] | 0.22 | 0.16 | 0.54 | 0.91 | 115.12 | 45.00 | 154.23 | 314.35 |

[(a)] Identical in this work and in Ramos et al. (2016); [(b)] Taken from Ramos et al. (2016); [(c)] This work.

**Table 4**
Regeneration and recycle solution.

| | Operating Cost (OF1) [$10^6$ €/year] | | | | | Freshwater Consumption (OF2) [$m^3$/h] | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | *e1* | *e2* | *e3* | *Total* | α | *e1* | *e2* | *e3* | *Total* | β |
| *MOO-GP*[(a)] | 0.19 | 0.06 | 0.54 | 0.79 | 0.13 | 20.00 | 20.00 | 122.8 | 162.80 | 0.48 |
| *MLSFG*[(a)] | 0.24 | 0.14 | 0.44 | 0.83 | 0.09 | 77.10 | 48.14 | 94.38 | 219.62 | 0.30 |
| *SLMFG*[(a)] | 0.19 | 0.13 | 0.39 | 0.71 | 0.22 | 20.00 | 20.00 | 20.00 | 60.00 | 0.81 |

[(a)] Taken from (Ramos et al., 2016); [(b)] Benefit over OP2 solution from this work (Table 3).

These formulations differ in the prioritization of objectives: The multi-objective optimization with goal programming (MOO-GP) formulation (Ramos et al., 2014) yields a Pareto optimal network solution with respect to a set of targeted objectives. The Single-Leader Multi-Follower (SLMF) formulation is a Game Theoretical approach. In Ramos et al. (2016) the leader is a single authority with the objective to minimize freshwater consumptions. The multiple followers are the enterprises in an EIP, minimizing their operational cost. The follower's optimization problems are introduced as constraints to the leader's problem. The Multi-Leader Single-Follower (MLSF) formulation switches the role of the enterprises and the authority, yielding a solution that prioritizes the economic objective function. The base water exchange model is identical in all works, so the network solutions remain comparable. The influence of different problem formulations is discussed in Ramos et al. (2016). The problem formulation in this work is effectively a cooperative one, since a global economic objective is minimized and each enterprise joins the collaboration if its own objective is at least not worsened.

### 6.1. Standalone and reuse cases

Table 3 provides the solutions to the standalone case for each enterprise (OP1). They coincide with those determined by Ramos et al. (2016), thus validating the correct implementation of the base model. The reuse case solutions differ only slightly in the global objectives ($0.95 \times 10^6$ €$year^{-1}$ and 314.35 $m^3h^{-1}$). This corresponds to benefits of 3% and 7% over the standalone case respectively. Solving OP2 leads to the same reduction in freshwater consumption but yields a lower global operating cost ($0.91 \times 10^6$ € $year^{-1}$) which corresponds to a reduction of 6% over the standalone case. This difference stems from the non-competitive formulation, enabling synergistic savings. It is evident that cooperative strategies have globally better outcomes, as demonstrated in the case of other green supply chains (Madani and Rasti-Barzoki, 2017).

It is important to note that each solution has an associated water distribution network. Since we are interested in targeting the benefits that are based in the objectives rather than the structure we omit the discussion of structural aspects. Once a satisfying solution has been found, the individual network can be investigated more in-depth.

It can be seen that even in the absence of a RU benefits can be achieved. The reference values for defining the benefits α and β in the following sections are the values obtained from solving OP2 (115.4 €$h^{-1}$ and 314.35 $m^3h^{-1}$).

**Table 5**
Regeneration units considered by Ramos et al. (2016) with limiting benefits.

| | Concentration $C^{out,fix}$ [ppm] | Cost $\gamma_u$ [€ $m^{-3}$] | $\alpha^{max}$ | $\beta^{max}$ |
|---|---|---|---|---|
| *RU1* | 15 | 0.850 | 0.286 | 0.809 |
| *RU2* | 20 | 0.695 | 0.337 | 0.809 |
| *RU3* | 30 | 0.540 | 0.365 | 0.740 |

### 6.2. Regeneration and recycle case

The integration of a RU to the system allows for further reduction of operational cost and freshwater consumption as can be seen in Table 4. Ramos et al. (2016) provide solutions to their MOO-GP, MLSFG and SLMFG formulations when integrating three RUs with the specifications given in Table 5. It can be seen that the most pessimistic solution is based in the MLSFG formulation. This solution corresponds to a state where the three leaders gain approximately equal benefit over the standalone case (14.5%, 13.5% and 14.0%). Their MOO-GP solution provides larger benefits in both objectives. However, it does not provide benefit to all enterprises, as *e3* does not benefit from the collaboration. The authors mention that this is due to the arbitrary choice of GP parameters, so tuning them could provide globally better solutions with fair distribution of benefits. Lastly, their SLMFG solution provides the highest benefits in both objectives while granting an economic benefit to each participating enterprise (31.9%, 19.4% and 25.1%). An organizing authority that imposes guides for minimizing the freshwater consumption will lead to synergistic benefits in both objectives.

The economic and environmental targeting problems have been solved using a full-factorial design on the RU specifications $c_{j,u}^{out,fix}$ and $\gamma$. Using the pinch point methodology, the upper bound for $c_{j,u}^{out,fix}$ can be determined to 150 ppm. Thus, the $c_{j,u}^{out,fix}$ range was covered from 0 to 150 ppm in 2 ppm increments, leading to 76 optimization problems per $\gamma$. Through trial and error, it was shown that no feasible solution with $\alpha \wedge \beta > 0$ can be found above 1.85 €$m^{-3}$. Thus, this design specification was covered from 0 to 1.85 €m $^{-3}$ in increments of 0.05 €$m^{-3}$, leading to 39 optimization problems per $c_{j,u}^{out,fix}$. As a result, a total of 2,964 problems per targeting problem had to be solved. A large amount of them (Fig. 5, dark blue area) were instantly determined to be infeasible.

Fig. 5 shows the resulting barrier plots for the economic and environmental targeting problems. The region of RU specifications leading to benefit ($\alpha \wedge \beta > 0$) is the same in both cases ($\alpha \wedge \beta = 0$). As previously indicated, the achievable benefit (in percent over reference case) is

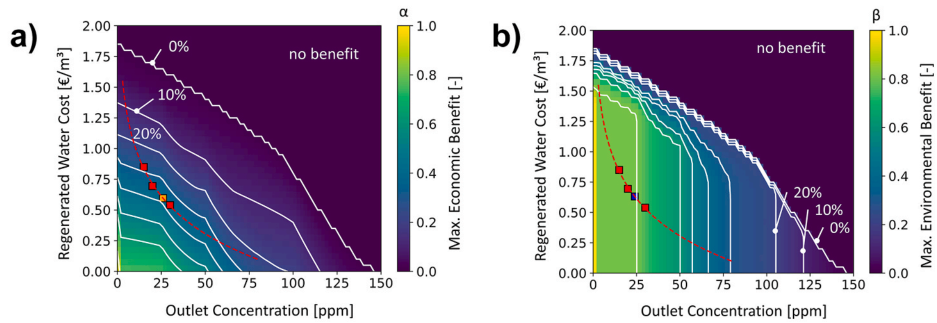


**Fig. 5.** Economic ($\alpha \geq 0$, $\beta = 0$) and environmental ($\alpha = 0$, $\beta \geq 0$) targeting maps for single-contaminant, multi-process case study. (■) RUs from Table 5; (▬▬▬) Cost curve regression through RUs ( $y = -0.443 \ln x + 2.039$ ); (■) Economically optimal RU; (■) Environmentally optimal RU.

generally larger for the environmental targeting problem. While the economic barriers follow a descending trend in permissible regenerated water cost for higher RU outlet concentrations, the environmental barriers follow a near linear descending trend with a limiting concentration where the barrier cuts off.

Depicted are also the RU specifications assumed by Ramos et al. (2016). The dashed curve is a regression through the three RUs, that approximates a cost function of treating water depending on the outlet concentration. This function is assumed to follow a logarithmic behavior with costs increasing steeply when approaching complete contaminant removal ($c_{j,u}^{out,fix} = 0\,ppm$). The main point to be noted is that with all of the RUs operating on their own a larger economic benefit (Table 5, $\alpha^{max}$) can be achieved than in the solutions from in Table 4. The maximum environmental benefit $\beta^{max}$ is the same as in the SLMFG solution, as this case corresponds to the situation where units *u1* ($c^{in,max} = 0$ ppm) in each enterprise are supplied by freshwater and the remaining units by reused or regenerated water. Only a hypothetical RU with full contaminant removal could further reduce the freshwater consumption to 0 $m^3h^{-1}$.

Using the cost regression curve in combination with the determined response surface, the optimal RU for each objective (Fig. 5) can be determined. As for the economically optimal RU an outlet concentration of 26 ppm corresponding to a treatment cost of 0.596 €$m^{-3}$ leads to an optimal economic benefit of 37.5%. In this scenario, the individual enterprise reductions are 11.5%, 37.1% and 57.8% respectively. Compared to the solutions in Table 4 enterprise *e1* has a smaller relative profit while enterprise *e3* benefits immensely from the cooperation. Under this consideration, a benefit sharing negotiation between the enterprises for a cooperative strategy could be favorable.

The environmentally optimal RU can be found on the plateau ranging from 0 to 24 ppm where the maximum environmental benefit is 80.9%. Logically, the optimal specification is then 24 ppm as this reduces both the treatment cost for the RU operator and increases the achievable economic benefit in the system. Considering that the optimal RU specification in both cases are 24 and 26 ppm a reasonable trade-off would be a guaranteed 25 ppm outlet concentration. Such a clear alignment of both objectives is not intrinsically granted and could be considerably different for other water systems.

Fig. 6 shows the feasible regions for a set of targets corresponding to the solutions in Table 4. As previously mentioned, this data can be employed by the different stakeholders for decision making. The three subfigures correspond to low, medium and highly ambitious targets. A RU operator can decide based on this information whether or not the market is attractive for its integration. In this case, the three RUs managed by the operator can be profitably integrated into the market.

The enterprises (and a political or managerial authority) can come together and analyze their inherent saving potential. First, the saving potential without integrating a RU is revealed. Then, negotiated targets

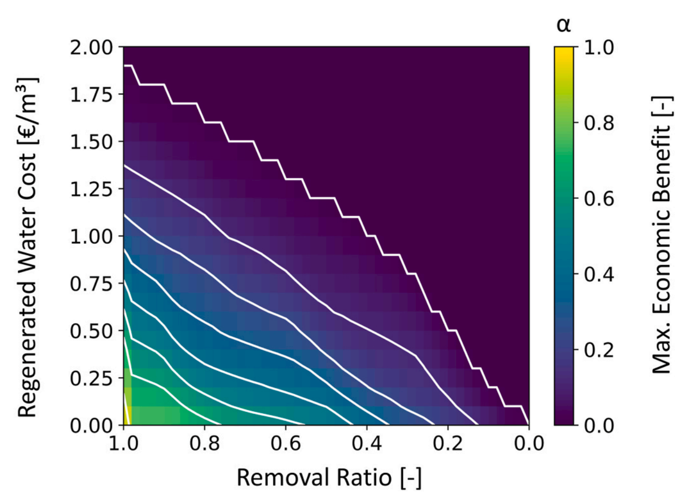


**Fig. 7.** Economic targeting maps for fixed removal ratio (RR) unit.

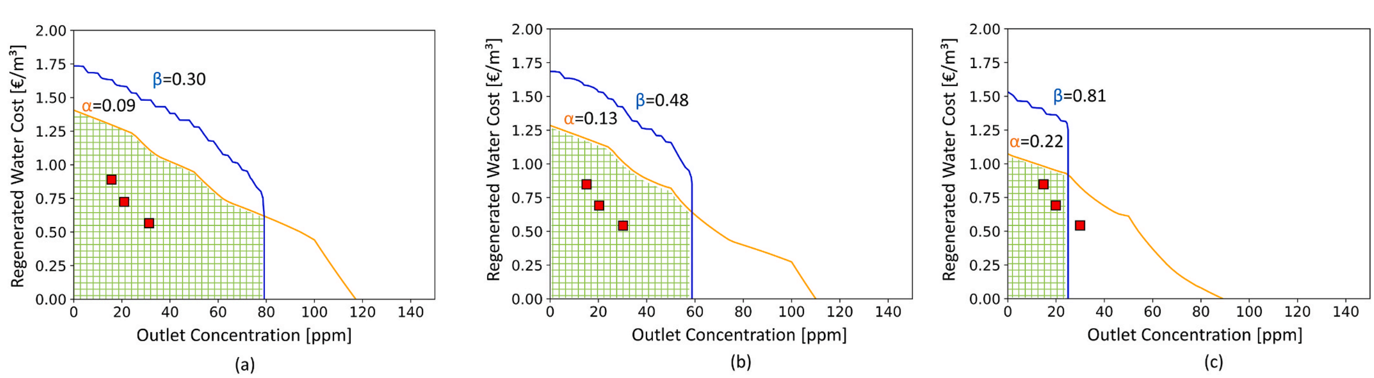


**Fig. 6.** Barriers for single RU systems to reach the targets obtained in the three solutions from Ramos et al. (2016) (see Table 3).

of different ambitiousness can be defined and the market can be screened for treatment companies that can meet these targets. Furthermore, this data can serve as a basis of negotiation between the enterprises.

### 6.3. RU removal ratio vs. concentration

Fig. 7 depicts the solution of the economic targeting OP3 when changing the fixed outlet concentration $c_{j,u}^{out,fix}$ assumption with a fixed removal ratio $\rho_{j,u}$. This substitution increases the problem difficulty considerably because the outlet concentration of the RU depends on the inlet concentration. The increased difficulty of optimizing water networks with fixed removal ratio RUs compared to RUs with a fixed outlet concentration is known (Parand et al., 2016) and the same difficulty applies to the presented methodology (see section 6.5). As a consequence, the number of design specifications to be evaluated is reduced to increments in removal ratio and regenerated water cost of 0.04 and 0.1 €m$^{-3}$ respectively (26 × 20 = 520 points). Despite the computational complexity, it is shown that the methodology can produce results for the alternative modeling choice (fixed removal ratio).

The discussion on the logic behind the modeling choice can be extended. In the context of water systems with regulated inlet, outlet and environmental discharge concentrations the policy of granting a certain (fixed) concentration of the regeneration unit is logical. Alternative strategies to deal with the optimization of water systems with higher fidelity models for the treatment process and a tailored solution approach is presented by Yang et al. (2014). The trade-off between increased computational expense and accuracy of the calculated solutions in larger scale networks such as EIPs or municipal water systems is yet to be discussed.

### 6.4. Piping cost

In a sensitivity analysis we vary the piping cost to see its effect on the barriers. Here, the source of uncertainty in the piping cost can stem both from (i) the uncertain specific piping cost (€/m) or (ii) the uncertain distance between the units (m). Further particular uncertainties could be considered, but they fall beyond the general scope of this work. Fig. 8 shows the maximum achievable α and β for a regenerated water cost of 0 €m$^{-3}$. It can be seen that, naturally, with increasing piping cost (δ from 0 to 0.25 €m$^{-3}$) less economic benefit can be achieved while the change in piping cost does not affect the environmental benefit. For a negligible piping cost (δ = 0 €m$^{-3}$) both objectives align perfectly. With increasing piping cost the feasible region for economic benefit becomes increasingly smaller until it vanishes at 0.25 €m$^{-3}$. Previously, a value of 0.02 €m$^{-3}$ has been assumed. Small variations in this assumption have little influence on the barrier but if the piping costs are considerably larger (e.g. for very large distances between the enterprises) the intrinsic saving potential through regeneration is cancelled. Therefore, it can be concluded that the application in EIPs is favorable due to the short distances between enterprises. But the methodology allows the expansion of the geographical limits of water exchange applied to different markets by revealing its potential.

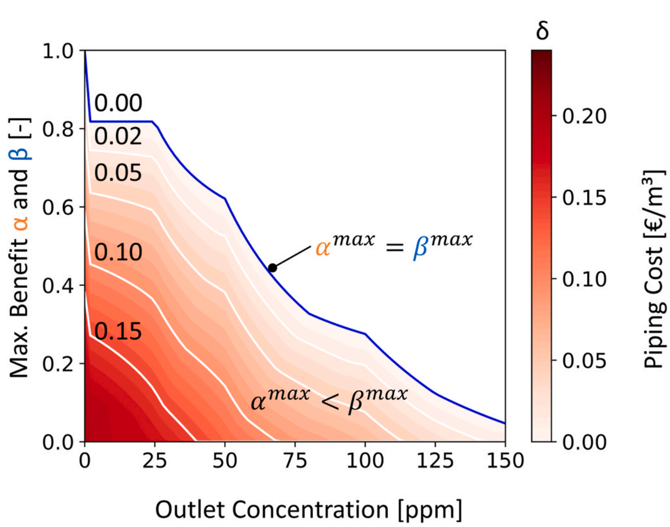


**Fig. 8.** Maximum economic and environmental benefit for varying piping cost. Cost of regenerated water set to 0 €m$^{-3}$.

### 6.5. Computational statistics

The number and types of equations are summarized in Table 6. The optimization problems are implemented in Pyomo, Python 3.8.3 and solved using the ANTIGONE MINLP general purpose solver through the GAMS 29.1 interface on a Windows 10 computer with an Intel Xeon Silver 4114 CPU 2.20 GHz and 128 GB DDR3 RAM. The large amount of OP3 problems were solved in parallel on the 20 available cores on the machine, each being assigned to a single core.

Fig. 9 illustrates the solution time for each optimization problem in the economic (9a) and environmental (9b) targeting of the fixed $c^{out}$ case. It can be seen that the non-benefit cases (α $^{max}$ = β$^{max}$ = 0) are usually identified and solved in less than 1s. In the more challenging situations the solver finds a solution with a relative optimality gap of 10$^{-5}$ in less than 100s for the economic targeting (3.57s average) and less than 500s for the environmental targeting (7.11s average). Using the 20 cores in parallel, the complete maps were determined in 30 min and 2h respectively. In the fixed removal ratio case (9c) the problem complexity increases considerably and in most of the benefit cases the solver runs until the maximum assigned runtime limit of 3,600s.

Certainly, tuning the general-purpose solver ANTIGONE parameters, applying smart bounding and initial points or other optimization tricks could speed up the solution procedure. However, fine tuning of the solution procedure and scaling considerations remain out of the scope of this contribution.

### 6.6. General remarks

The presented methodology is general enough to be able to deal with multiple-contaminant systems, but in this case the generation of similar 2D/3D targeting maps becomes more complex as these would be multidimensional. With each added contaminant, a degree of freedom is added to the model and covering its complete influence increases the number of necessary optimization problems to be solved exponentially. Identifying single or few critical contaminants in the water system could reduce the number of optimization problems to be solved and speed up the targeting procedure (Chin et al., 2021).

The same logic of increasing necessary optimization problems applies for the investigation of multiple RUs with independent costs. The latter problem can be tackled by considering multiple RUs with different treatment modes and costs as single RU with a cost distribution as demonstrated in section 6.2. This works as long as the RUs are managed

**Table 6**
Number and type of equations after pre-processing for the three optimization problem types considered.

| | Standalone (OP1) | Reuse (OP2) | Regeneration and Recycle (OP3) |
|---|---|---|---|
| Continuous Variables | 146 | 212 | 222 |
| Binary Variables | 442 | 500 | 527 |
| Linear Equations | 91 | 100 | 83 |
| Nonconvex Nonlinear | 140 | 204 | 249 |
| Bilinear Terms | 342 | 360 | 654 |

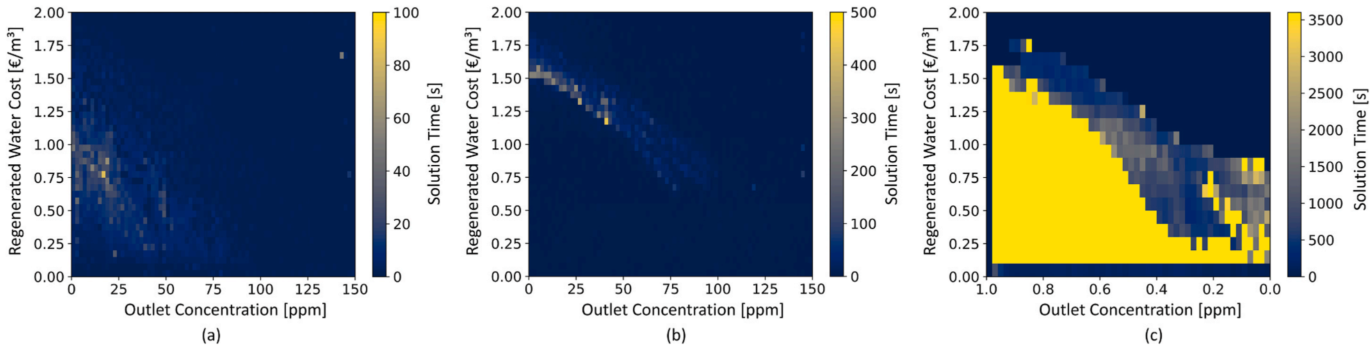


**Fig. 9.** Solution time of individual optimization problems for the different modeling assumptions. Color scale on each Figure is non-uniform to better visualize differences in time for each case.

by a single operator and no competition between RU operators takes place.

As indicated in Section 6.5, for the selected case study and fixed $c^{out}$ case the computational time is manageable, despite the large amount of optimization problems. However, more complex water systems and the alternative modeling assumption (fixed removal ratio) may raise the need to restrict the investigated RU design specification region or apply other strategies to reduce the amount of individual optimization problems to be solved. For instance, an adaptive sampling strategy focusing on the areas of interest ($\alpha > 0,\ \beta > 0$) could be used (Garud et al., 2017). Smarter adaptive sampling with surrogates approximating the response surface can greatly reduce the computational expense for creating the barrier plots.

## 7. Conclusions

This work contributes to fostering circular economy in water markets with a novel holistic approach and a related methodology able to identify and quantify the barriers preventing the achievement of targeted economic and environmental benefits in water systems through the integration of water regeneration units. The advantages of this methodology are illustrated through its application to a case study from the literature, to reveal and quantify the benefits that can be achieved through a cooperative strategy over the non-cooperative formulations: targeting to the same environmental benefit, the higher economic incentive of the cooperative solution favors its practical implementation. The application to a benchmark case study from the literature reveals a potential economic benefit of 37.5% and a freshwater reduction of 80.9% over the case without regeneration units. Moreover, a limiting piping cost of 0.25 €m$^{-3}$ for profitable integration of an RU has been identified in a sensitivity analysis.

The proposed methodology can determine the response surfaces to the economic and environmental targeting problems and makes use of them to solve mixed targeting problems. We discuss and provide guidelines and indications on how this data can be employed by the different stakeholders and on how to support the decision-making process to achieve targeted development goals.

Using a full-factorial design to obtain the required response surfaces is computationally very expensive. Thus, future efforts will be directed towards reducing the amount of necessary optimization problems to approximate the response surfaces with adequate precision in a reasonable time, and enabling the application of the methodology to more complex (multi-component, multi-process) systems, as well as addressing the full circularity of the water market including the valorization and recycling of water contaminants. In spite of these open issues, we presented a rigorous and flexible methodology that can be applied by decision makers in the water market to develop more sustainable solutions.

## CRediT authorship contribution statement

**Fabian Lechtenberg:** Conceptualization, Methodology, Software, Data curation, Writing – original draft, Visualization. **Ana Somoza-Tornos:** Conceptualization, Writing – review & editing. **Antonio Espuña:** Conceptualization, Writing – review & editing, Supervision, Project administration, Funding acquisition. **Moisès Graells:** Validation, Writing – review & editing, Supervision, Project administration, Funding acquisition.

## 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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Fig. 1 and the graphical abstract were made with icons designed by Freepik, Smashicons and DinosoftLabs from www.flaticon.com

## Notation

*Abbreviations*

| | |
|---|---|
| EIP | Eco-industrial park |
| MLSFG | Multi-leader single-follower game |
| MOO-GP | Multi-objective goal programming |
| OF | Objective function |
| OP | Optimization problem |
| RU | Regeneration unit |

SLMFG Single-leader multi-follower game

*Parameters*

| | |
|---|---|
| $a_d$ | Slope in linear interval |
| $b_d$ | Intercept in linear interval $m^3/h$ |
| $C^{env}$ | Discharge cost €/$m^3$ |
| $C_f$ | Freshwater cost of source f €/$m^3$ |
| $C^{pipe}$ | Piping cost €/$m^3$ |
| $C^{reg}_{u'}$ | Regeneration cost of unit u' €/$m^3$ |
| $c^{in,max}_{j,u}$ | Max. inlet contamination of contaminant j in unit u ppm |
| $c^{out,max}_{j,u}$ | Max. Outlet Contamination of contaminant j in unit u ppm |
| $c^{out,fix}_{j,u}$ | Fixed outlet contamination of RU u ppm |
| $c_{j,f}$ | Freshwater contamination ppm |
| $m_{j,u}$ | Contamination load of unit u gh-1 |
| $Q^{max}_u$ | Maximum Inlet Flow of unit u $m^3/h$ |
| $Q^{min}_u$ | Minimum Inlet Flow of unit u $m^3/h$ |
| $\rho_{j,u}$ | Removal ratio of RU u |

*Variables*

| | |
|---|---|
| $c^{out}_{j,u}$ | Outlet contamination of unit u ppm |
| $c^{in}_{j,u}$ | Inlet contamination of unit u ppm |
| $y_{u,u'}$ | Active connections |
| $y_{f,u}$ | Active freshwater connections |
| $y_{u,d}$ | Active linearization interval |
| $OF1_e$ | Economic objective function €/h |
| $OF2$ | Environmental objective function $m^3/h$ |
| $Q^{env}_u$ | Environmental discharge flow $m^3/h$ |
| $Q_{f,u}$ | Freshwater flowrate $m^3/h$ |
| $Q^{inter}_{u',u}$ | Water flow between units $m^3/h$ |
| $Q^{in}_u$ | Inlet flow of unit u $m^3/h$ |
| $Q^{out}_u$ | Outlet flow of unit u $m^3/h$ |
| $\alpha$ | Economic benefit over reuse case |
| $\beta$ | Environmental benefit over reuse case |

*Sets*

| | |
|---|---|
| e ∈ | E Enterprises |
| f ∈ | F Freshwater sources |
| j ∈ | J Contaminants |
| u ∈ | U Units |
| $d \in D$ | Linearization set |

## Appendix A

*Water Balance*

Fig. 3 depicts the mass balance of a general water using unit. The inlet and outlet balances are given by Equations (A1) and (A2):

$$Q^{in}_u = \sum_{u' \in U_{RU},\ U_e} Q^{inter}_{u',u} + \sum_{f \in F} Q_{f,u}\ \forall u \in U_{RU},\ U_e \tag{A1}$$

$$Q^{out}_u = Q^{in}_u = \sum_{u' \in U_{RU},\ U_e} Q^{inter}_{u,u'} + Q^{env}_u\ \forall u \in U_{RU},\ U_e \tag{A2}$$

where $Q^{in}_u$ is the inlet flowrate of unit $u$ consisting of the interchange flowrates $Q^{inter}_{u',u}$ from other units $u'$ to $u$ and freshwater sources $f$. Assuming there is no water loss, the inlet flowrate equals the outlet flowrate $Q^{out}_u$ which consists of the flowrates distributed from unit u to other units u' ($Q^{inter}_{u,u'}$) and to the environment ($Q^{env}_u$).

In the case of water users, input flowrates are limited by upper and lower bounds ($Q^{max}_u$ and $Q^{min}_u$) as shown in Equation (A3).

$$Q^{\min}_u \le Q^{in}_u \le Q^{\max}_u\ \forall u \in U_{RU},\ U_e \tag{A3}$$

*Contaminant Balance*

Contaminants are substances in the water that can have a negative impact on the environment, health or process performance (e.g. oils and fats, feces, traces of medication …). Their inlet balance is stated in Equation (A4):

$$Q_u^{in} \cdot c_{j,u}^{in} = \sum_{u' \in U_{RU},\ U_e} Q_{u',u}^{\text{inter}} \cdot c_{j,u'}^{out} + \sum_{f \in F} Q_{f,u} \cdot c_{j,f} \ \forall u \in U_{RU},\ U_e \ \forall j \in J \tag{A4}$$

The inlet concentration $c_{j,u}^{in}$ is determined by the water streams coming from other units ($c_{j,u'}^{out}$) and the freshwater ($c_{j,f}$). Depending on the type of water using unit the outlet balance takes different forms. For regular water using units $u$ it takes the form of Equation (A5) where $m_{j,u}$ is the amount of contaminant $j$ that is entering the water stream in unit $u$ (e.g. contamination in cleaning water).

$$c_{j,u}^{out} = c_{j,u}^{in} + \frac{m_{j,u}}{Q_u^{in}} \ \forall u \in U_e \ \forall j \in J \tag{A5}$$

*Structure*

Fig. 2 (c) depicts the water system superstructure. Feasible connections between units are defined by a binary parameter $x_{u,u'}$ in Equation (A6).

$$Q_{u,u'}^{\text{inter}} \cdot \left(1 - x_{u,u'}\right) = 0 \ \forall u, u' \in U_{RU}, U_e \tag{A6}$$

Active connections are specified by the binary variable $y_{u,u'}$ in Equation (A7).

$$Q_{u,u'}^{\text{inter}} \cdot \left(1 - y_{u,u'}\right) = 0 \ \forall u, u' \in U_{RU}, U_e \tag{A7}$$

Freshwater connections are defined the same way in Equations (A8) and (A9).

$$Q_{f,u} \cdot \left(1 - x_{f,u}\right) = 0 \ \forall u \in U_e \ \forall f \in F \tag{A8}$$

$$Q_{f,u} \cdot \left(1 - y_{f,u}\right) = 0 \ \forall u \in U_e \ \forall f \in F \tag{A9}$$

Discharging water to the environment may be avoided for some specific Units (e.g. RUs) through the parameter $z_u^{env}$ in Equation (A10).

$$Q_u^{env} \cdot \left(1 - z_u^{env}\right) = 0 \ \forall u \in U_e \tag{A10}$$

## Appendix B

The nonlinear term $(Q_{u',u}^{inter})^{\psi}$, where $\psi = 0.6$, in the objective function has been replaced with a piecewise linear approximation $Q_u^{reg}$:

$$Q_u^{reg} = \sum_d y_{u,d} \cdot \left(a_d \cdot Q_{u',u}^{\text{inter}} + b_d\right) \ \forall u \in U_e \ \forall u' \in U_{RU} \tag{B1}$$

To that end, a new set for the discrete intervals $d \in D$ must be introduced. It was found that 20 intervals in the range 0–500 $m^3h^{-1}$ lead to a sufficient representation of the nonlinear function (see Figure B1). The coordinates of the discretization points (red squares) were determined through minimization of the area between the piecewise approximation and the power function. The binary variable $y_{u,d}$ indicates which interval $d$ is active for which unit $u$:

$$\sum_d y_{u,d} \cdot Q_d^{lower} \le Q_{u',u}^{\text{inter}} < \sum_d y_{u,d} \cdot Q_d^{upper} \ \forall u \in U_e \ \forall u' \in U_{RU} \tag{B2}$$

This simplification speeds up the optimization procedure while there is little change in the observed barriers.

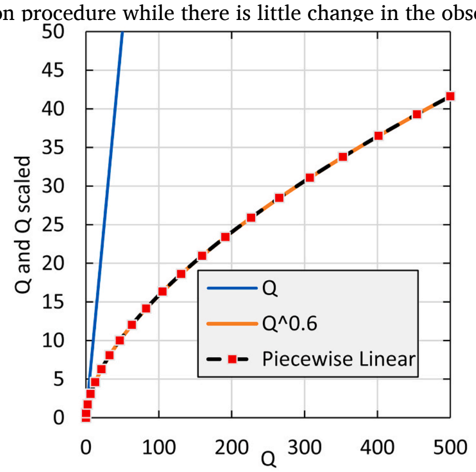


**Fig. B1.** Piecewise linearization with 20 intervals of the nonlinear term ${Q_{u',u}^{inter}}^{0.6}$.

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