Water integration in eco-industrial parks using a multi-leader-follower approach

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A B S T R A C T

The design and optimization of industrial water networks in eco-industrial parks are studied by formulating and solving multi-leader-follower game problems. The methodology is explained by demonstrating its advantages against multi-objective optimization approaches. Several formulations and solution methods for MLFG are discussed in detail. The approach is validated on a case study of water integration in EIP without and with regeneration units. In the latter, multi-leader-single-follower and single-leader-multi-follower games are studied. Each enterprise's objective is to minimize the total annualized cost, while the EIP authority objective is to minimize the consumption of freshwater within the ecopark. The MLFG is transformed into a MOPEC and solved using GAMS® as an NLP. Obtained results are compared against the MOO approach and between different MLFG formulations. The methodology proposed is proved to be very reliable in multi-criteria scenarios compared to MOO approaches, providing numerical Nash equilibrium solutions and specifically in EIP design and optimization.

Keywords:
Eco-industrial parks
Multi-leader-follower game
Nash equilibrium
Multi-objective optimization
MPCC
Game theory

1. Introduction

During the last few decades, industrialization has contributed to rapid depletion of natural resources such as water and natural gas. Consequently, there is a real need for industries to ensure minimum natural resources consumption, while maintaining good production levels. In particular, industrial development is often linked to the use of high volumes of freshwater (Boix et al., 2010, 2011). In order to work towards global environmental preservation while increasing business success, the concept of industrial ecology has emerged (Boix et al., 2015). This concept, which is directly linked to sustainable development, aims at engaging separate industries, geographically closed enough, in a collective approach so that exchanges of raw matter, by-products, energy and utilities (Chertow, 2000) are maximized. Indeed, the most widespread manifestations of these kinds of industrial symbiosis are eco-industrial parks (EIP). A definition widely accepted of EIP is "an industrial system of planned materials and energy exchanges that seeks to minimize energy and raw materials use, minimize waste, and build sustainable economic, ecological and social relationships" (Boix et al., 2015; Montastruc et al., 2013; Alexander et al., 2000). As it can be highlighted, a basic condition for an EIP to be economically viable is to demonstrate that benefits of each industry involved in it by working collectively is higher than working as a stand-alone facility.

Boix et al. (2015) highlighted the lack of studies dealing with optimization in order to design optimal configuration of an EIP. However, it is important to develop methodologies able to design an EIP where each industry has an effective gain compared to the case where they operate individually, by also taking into account environmental concerns. Among EIP design studies, water-using network is the most common type of cooperation modelled in literature (Boix et al., 2015). In this kind of studies, the case is often solved as a water-allocation problem through a superstructure-based model where water has to be distributed, treated and discharged in an optimal way between the process units of each enterprise/company involved in the EIP.

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Nomenclature

Latin symbols

nl	number of leaders
L	index set of leaders
x_i	decision variables of leader i
x_{-i}	decision variables of other leaders
w	decision variables of the follower
f	objective function of leader/leaders
g	inequality constraints of leader/leaders
z	objective function of the follower
m	inequality constraints of the follower
np	number of processes per enterprise
P	index set of processes
nep	number of enterprises
EP	index set of enterprises
nr	number of regeneration units
R	index set of regeneration units
M	contaminant load
$Cmax^{in}$, $Cmax^{out}$	maximum contaminant concentration allowed in inlet/outlet of processes
C^{out}	outlet concentration of contaminant in regeneration units
$Fpart$	water flow between different processes
Fw	freshwater inlet flow to processes
$Fproreg$	water flow from processes to regeneration units
$Fregpro$	water flow from regeneration units to processes
$Fdis$	water processes to the discharge
$\min f$	minimum flowrate allowed
AWH	annual EIP operating hours

Greek symbols

ν	Lagrange multipliers relative to m
μ	Lagrange multipliers relative to g
ξ	Lagrange multipliers relative to s
$\pi, \nu, \eta, \tau, \varphi$	slacks to inequalities of Prob. 7
α	purchase price of freshwater
β	polluted water discharge cost
δ	polluted water pumping cost
	regenerated water cost
	power associated to γ

Modelling EIPs based on water-exchange networks is somewhat a complex problem, since, depending on the number of enterprises and processes, a model with thousands of variables, constraints and disjunctions has to be solved. On the other hand, it is obvious that the design of EIPs through mono-objective optimization it is not trivial, since to choice a single objective function is almost impossible due to the size of the manifold of the possible objective functions. As aforementioned, the main aim of industrial symbiosis is to minimize pollution and resources utilization while maximizing each company's gain. For instance, by using a mono-objective optimization approach and minimizing the EIP total annualized cost do not necessarily agree with environmental objectives. Indeed, it is due to the latter that these kind of problems are better tackled with a multiobjective optimization (MOO) approach (Boix et al., 2015; Montastruc et al., 2013; Boix and Montastruc, 2011).

Recently, Boix et al. (2012) developed a multi-objective optimization strategy based on the ε-constraint method applied to the case of a water network in an EIP under several scenarios. The interest of dealing with multiobjective optimization is to build a Pareto front in which several optimal solutions are available; then, an a posteriori tool of multi-criteria decision making is further applied. In the aforementioned work, three antagonist objective functions were taken into account: freshwater consumption, number of connections and total regenerated water-flowrate. On the other hand, a posterior work of Montastruc et al. (2013) has explored the flexibility of the designed EIPs by changing parameters related to processes. The authors have also analyzed different indicators to test the EIP profitability. Then, a later extension of this work was conducted by Ramos et al. (2015): they employed a multiobjective optimization approach by minimizing each enterprise capital cost by using goal programming (GP). This approach is based on a recent study where GP has been proven to be a very reliable method to design industrial water networks following multiple antagonist objective functions (Ramos et al., 2014).

Indeed, previous studies have widely explored Pareto front generation approaches but some numerical problems were encountered especially when a very large number of binary variables are involved. In most cases, choosing the bounds for generating methods (e.g. ε-constraint method) is a non-trivial task, and the choice of these bounds is important because if they are not well chosen the solver may not succeed into obtaining a feasible solution. Furthermore, if a solution is found it remains a very long and tedious computational task. That is why a GP approach shows more affinity with EIP design. However, Ramos et al. (2015) demonstrated that in different scenarios and by tuning different optimization parameters (e.g. weight factors associated with the objective functions) one company is favoured compared to the others. Although optimal solutions are intermediate and satisfying in terms of individual costs, it is of great interest to

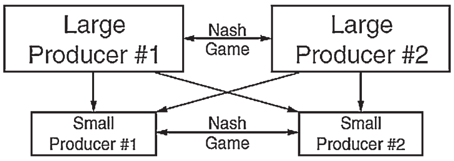

Fig. 1. Example of a multi-leader-follower game (Leyffer and Munson, 2010).

Table 1
Summary of the state of the art.

Article	Number of enterprises	Number of processes per enterprise	Regeneration units	Comments
Lou et al. (2004)	2	1	No	Nash equilibrium between 2 enterprises with sustainability and profit objectives. Each enterprise has its own process already optimized.
Chew et al. (2009)	3	5	No	A posteriori game theory approach to choose the best integration scheme among alternatives obtained by classical optimization.
Aviso et al. (2010)	4	1	No	SLMFG fuzzy optimization. Each enterprise has its own process already optimized.
This work	3	5	Yes	MLSFG/SLMFG with and without regeneration units. The optimal configuration within each enterprise is taken into account. Different models and solution methods explored.

obtain more balanced solutions so that each enterprise/company is satisfied at the same time and moreover, by minimizing freshwater consumption in order to insure the environmental performance of the EIP.

An interesting alternative particularly adapted to the optimal design of EIP is the Game Theory approach and most particularly the concept of the generalized Nash equilibrium problem (GNEP). In fact, an EIP can be seen as the congregation of different non-cooperative agents (i.e. the enterprises) which aim at minimizing their annualized operating costs and an EIP authority whose aim is to minimize resources consumption (e.g. freshwater). This kind of non-cooperative game is very interesting for the concepts of EIP, since the main barrier to integrate an EIP for industry is the issue of confidentiality between enterprises and this approach could be very promising to overcome this problem. In fact, by introducing an impartial authority (or regulator) whose role is to collect all data necessary to design the EIP, enterprises involved would be able to keep confidential data, without the need to share them with the other companies of the park. Indeed, it could be useful to overcome the difficulties linked to information exchanges between companies in an EIP. However, it is important to deal with an authority that attends to minimize environmental impacts of the EIP. In the context of non-cooperative games, a single solution for the design of an EIP can be achieved and proposed by obtaining a Nash equilibrium. In this solution, no agent can unilaterally deviate in order to improve its pay-off (Aussel and Dutta, 2008), that means, in our context and compared to the Pareto front approach, that no enterprise will be in interested in changing his strategy. In fact, the Nash equilibrium is the solution driven by the set of strategies in which each player has chosen an optimal strategy given the strategies chosen by other players. The latter is clearly a crucial point in the design of an optimal EIP.

The kind of problem described above (i.e. enterprises with an EIP authority/regulator) can be modelled generally as a multi-leader-follower game where the role of leaders and followers depends on the priorities of the EIP, as it will be explained in the subsequent sections. This kind of approaches is widely studied for modelling of deregulated electricity markets (Hu and Ralph, 2007; Hobbs et al., 2000; Aussel et al., 2013). In this kind of games, leaders make simultaneous decisions and the followers react to these decisions (Leyffer and Munson, 2010). In other words, the followers play a Nash game between them so as the leaders. Fig. 1 shows an example of the general case of a multi-leader-multi-follower game in which two large electricity producers act as the leaders, with a number of smaller producers acting as the followers play a Nash game.

2. Previous studies

On the subject of EIP or even industrial symbiosis, Nash games, Multi Leader Follower Game (MLFG) and even game theory are very little studied. For instance, Lou et al. (2004) studied the possible conflicts of profit and sustainability objectives of the member entities by treating the EIP as a Nash game. This methodology was then applied to a very simple case with two enterprises by taking into account uncertainty. In fact, they obtained conflicting results between the aforementioned objectives by evaluating the system. Then, Chew et al. (2009) developed a game theory approach for the decision making process for water integration in an EIP. Nevertheless, the game theory approach was employed a posteriori, i.e. in the decision making process after the optimization step. In this study, different configurations of EIP's are obtained by classical optimization and then, the different integration schemes were evaluated regarding Nash equilibrium. Finally, Aviso et al. (2010) developed a single leader-multi follower game (SLMG) model with fuzzy optimization in order to model water exchange in EIP. The methodology is then evaluated in a medium-sized case study and under different scenarios. Table 1 summarizes the aforementioned state of the art. As it can be seen, this work deals with both MLSFG/SLMFG approaches for the design of EIP, in which at least the former, to the best of authors' knowledge, is an unexplored area of research regarding the design of EIP or even in any domain of process engineering. The aim of this work is to develop an alternative methodology to multi-criteria optimization generally used in the field of process engineering, by applying the methodology in an industrial ecology context. First, the MLSFG is formulated and solved in an optimization manner, and algorithmic, modelling and reformulations issues are discussed alongside. Then, it is demonstrated the power of such formulations by comparing them with MOO methodologies with a case study of considerable size where the consideration

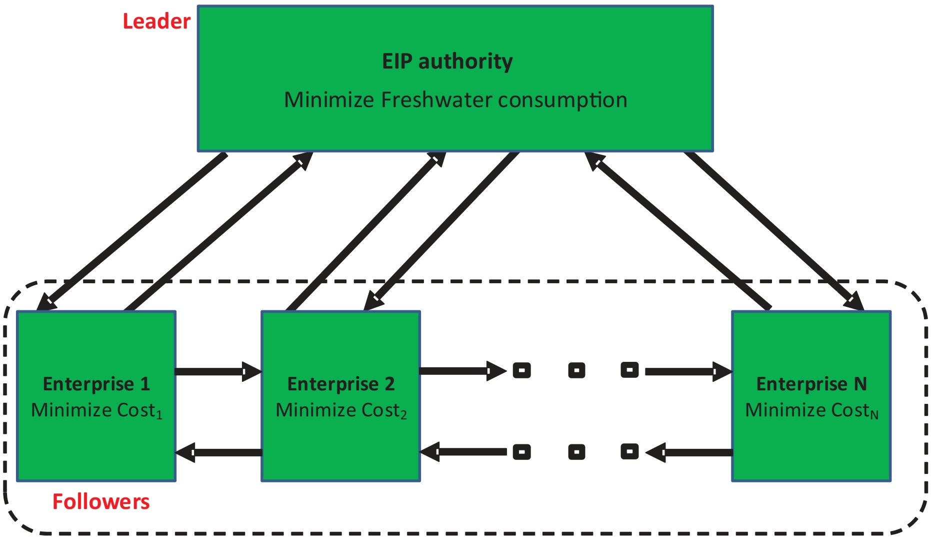

Fig. 2. General scheme of the proposed SLMFG.

of regeneration units is included. It is also important to specify that the optimal design of each plant is taken into account in the model. The latter is a fundamental point when designing EIP, since by first optimizing each enterprise and then by optimizing the EIP like in Lou et al. (2004) several optimal solutions could be discarded. In the subsequent sections, the MLFG approach is explained in detail, as well as different formulations, models for water integration with and without regeneration units and solution methodologies. Successively, results for each one of the case studies are presented, and comparisons with respective MOO results are made. Solving MLFG is a rather difficult task (Aussel and Dutta, 2008; Leyffer and Munson, 2010; Pang et al., 2005), and the modelling has to be accomplished very carefully and on the other side, solution methodologies have to be carefully chosen and tuned. Finally, it is important to highlight that large-scale MLFG models such as those addressed in this work have never been treated in literature before, to the best of authors' knowledge. Multi-leader-follower game approach

In order to obtain a solution for the kind of systems as EIPs are, where heavy interactions exist and where each entity is biased by their own interests, game theory is a viable tool for decision-making. As aforementioned, in Nash games, players make simultaneous optimal decisions given the optimal strategies of other players. Indeed, Nash equilibrium denotes the state where all the casual forces internal to the system balance each other out (Lou et al., 2004), and no player can improve its gain by unilaterally changing his strategy. By solving a Nash game, it is possible to obtain this kind of solution by definition. On the contrary, by considering the problem as a MOO problem, an ulterior decision-making procedure has to be successfully applied in order to obtain a solution where all participants are satisfied by the solution, as demonstrated by Ramos et al. (2014). If the participant is not satisfied with the solution, another solution has to be chosen by the decision maker from the pool of solutions or another solution has to be generated taking into account that preferences of the participants are known. In contrast, Nash games do not need to have information on participants' preferences. It is important to note that obtaining a solution with MOO that satisfies all participants is a very difficult task, and even impossible for certain cases (Ramos et al., 2015). Moreover, the case of MLSFG is impossible to model by MOO if leaders' optimal responses are unknown, which is almost always the case.

2.1. *Authority/regulator's design of an EIP and game theory approach*

The introduction of an authority/regulator to the design of viable water networks in EIP is an interesting alternative to overcome the confidentiality problem on one hand, and on the other hand, to solve the problem of equilibrium benefits of the players involved. In fact, the latter can be modelled as a MLSFG where the leaders are the enterprises whereas the EIP authority represents the only follower or as a SLMFG, when the roles are inversed. The choice between these different formulations depends on the priorities of the EIP.

The design of EIP water network by MLFG consists in near-located enterprise process plants that are subjected to regulations implemented in the park. Each enterprise has its own processes, and each process requires a specific water both in quantity and quality in order to operate. Moreover, each process produces a certain amount of wastewater, given its contaminant flowrate and an upper bound on outlet quality. In this particular case, only one contaminant is taken into account for the sake of simplicity. Each enterprise has access to water regeneration units, shared within the EIP.

At this point, it is important to note that in the MLFG approach the choice of leaders and followers is crucial in the problem formulation. As it will be explained later in terms of modelling and results, this choice changes completely the nature of the problem: On one hand, it can be assumed that enterprises act as followers and the authority as the lone leader (SLMFG) or vice versa (MLSFG). It is assumed that in the case of SLMFG the enterprises aim to minimize their total annualized cost, given the minimum flowrate consumption in the EIP, determined by the authority. This is in fact the same game as the one proposed by Aviso et al. (2010). A general scheme of the SLMFG proposed is shown in Fig. 2.

On the other hand, the game may be formulated as a MLSFG, where the EIP authority aims to minimize the total freshwater consumption, given the recycle and reuse of wastewater inside each enterprise and between enterprises, which minimizes their individual operating costs. A general scheme of the MLSFG proposed is shown in Fig. 3.

By changing the nature of the game as stated above, the priorities of the EIP are shifted. Indeed, in the latter case enterprises operating cost is predominant compared to total freshwater consumption and vice versa in the former case. In fact, in the MLSFG freshwater consumption

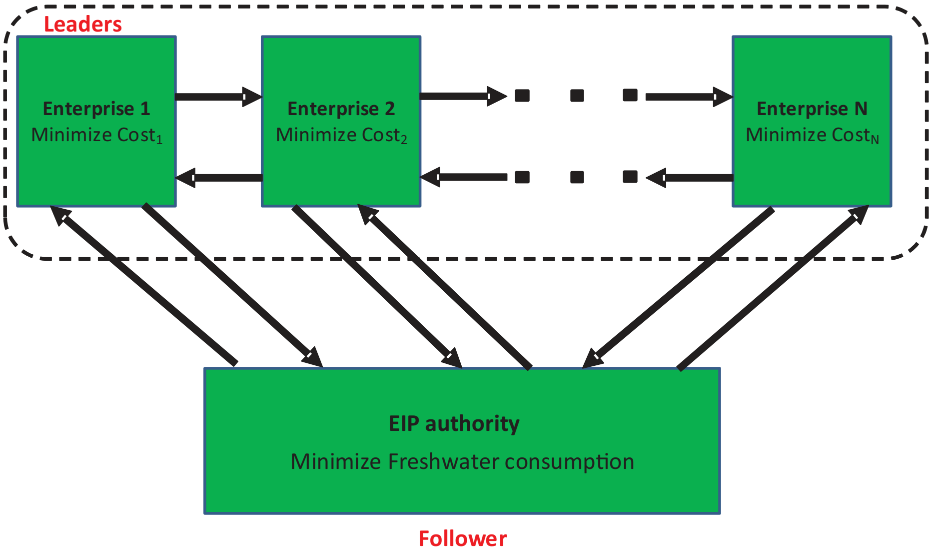

Fig. 3. General scheme of the proposed MLSFG.

is minimized only after each enterprise operating cost is minimized following the Nash game between the leaders. On the contrary, in the SLMFG each enterprise operating cost is minimized subject to a minimal total consumption of freshwater. These two formulations may be seen, the latter as a formulation where enterprises' revenues have priorities and the former as a formulation where environmental and sustainability issues are the priority. Clearly, the solutions obtained by both formulations are almost never the same. In consequence, it is self-understood that priorities have to be carefully chosen by the modeller or may be self-imposed by the problem.

Given the latter structures, we now proceed to formally present each one of the game formulations. MLSFG is presented first, since it is considerably more complicated than the SLMFG case.

2.2. Multi-leader single-follower game formulation

2.2.1. Bi-level model

A MLSFG has the following formal definition, without loss of generality (Aussel and Dutta, 2008; Leyffer and Munson, 2010; Kulkarni and Shanbhag, 2014):

Let $nl \geq 1$ be the number of leaders, and denote by $L = \{1, \ldots, nl\}$ the index set of leaders. Let x_i, $i \in L$ be the decision variables of leader i, x_{-i} the decision variables of other leaders. Let w be the vector of variables of the follower. The optimization problem solved by each leader i is the following Prob. 1:

$$\begin{array}{ll} \min\limits_{\substack{x_i \geq 0 \\ w}} & f_i(x_i, w, x_{-i}) \\ \text{subject to} & \left\{ \begin{array}{l} g_i(x_i, w, x_{-i}) \geq 0 \\ w \ \ \text{solves}: \\ \left. \begin{array}{l} \min\limits_{w \geq 0} \ \ z(x_i, w, x_{-i}) \\ s.t. \left\{ m(x_i, w, x_{-i}) \geq 0 \right. \end{array} \right\} (PF) \end{array} \right. \end{array} \qquad \text{(Prob. 1)}$$

Each leader minimizes his own objective f_i with respect to x_i subject to his inequality constraints g_i which are different for each leader. Moreover, the solution of each leader's problem is constrained to also be solution of follower's problem, which consist on minimizing z with respect to w subject to follower's inequality constraints m. Indeed, leaders play a Nash game between them, parameterized by the follower's problem.

It is very important to note that in the formulation shown in Prob. 1, follower's response is common among leaders, i.e. each leader makes two decisions: his strategy (x_i) and his conjecture about the solution of the follower (w). On the other hand, proving uniqueness of a solution to the MLSFG and even finding a solution is a very difficult task, given that each leader optimization problem is non-convex (Aussel and Dutta, 2008; Leyffer and Munson, 2010; Kulkarni and Shanbhag, 2014). In general, for a given $x_i, \forall i \in L$, it does not exist unicity of the conjecture w of problem (PF). Furthermore, it is well documented (Pang et al., 2005; Kulkarni and Shanbhag, 2014) that follower's decision variables status as common in each leader optimization problem is a non-negligible complication in order to solve such a problem, which may even condition the problem to not have an equilibrium solution at all.

Nevertheless, Kulkarni and Shanbhag (2014) proposed a shared-constraint approach for MLFG in which the solution space is enlarged in order to allow more games to have equilibrium solutions. In fact, through the shared-constraint approach Kulkarni and Shanbhag (2014) showed that under certain circumstances there exist links between the modified and the original problem (Prob. 1). This kind of approach is very important to the problem presented in this study and is in fact the formulation employed in this work.

Let Prob. 1 be the equivalent of the ε formulation, i.e. the classical formulation of a MLFG, denoted by Kulkarni and Shanbhag (2014). The modification proposed by the latter authors, consists in the following modification of the optimization problem Prob. 1 for each leader *i:*

$$\begin{aligned} \min_{\substack{x_i \geq 0 \\ w_i}} \quad & f_i(x_i, w_i, x_{-i}) \\ \text{subject to} \quad & \begin{cases} g_i(x_i, w_i, x_{-i}) \geq 0 \\ \forall k \in L, w_k \ \text{ solves :} \\ \left.\begin{array}{l} \min\limits_{w_k \geq 0} \quad z_k(x_k, w_k, x_{-k}) \\ s.t. \left\{ m_k(x_k, w_k, x_{-k}) \geq 0 \right. \end{array}\right\} (PF_k) \end{cases} \end{aligned} \tag{Prob. 2}$$

In Prob. 2 it is to be noted in first place, that each variable of the follower is duplicated for each leader i.e. they inherited the *i* index. Indeed, each leader does his own conjecture about the follower's equilibrium. On the other hand, the modification entails that each leader is now constrained by the problem of the follower regarding both his own conjecture as other leaders' conjectures, i.e. follower's problems and variables are now duplicated for each leader, denoted by index *k*. Then, the *i*th leader problem is parameterized by the decision of other leaders, i.e. x_{-i} and other leaders' conjectures about follower's equilibrium, i.e. w_{-i}. The formulation in Prob. 2 is the so called Nash game with shared-constraints, which corresponds to formulation ε^{ae} (*all equilibrium*) in Kulkarni and Shanbhag (2014). The result is that for any *i*, w_i satisfies the same constraints as in Prob. 1, but x_i is constrained by additional constraints in Prob. 2. In fact, Kulkarni et al. successfully proved that formulation ε^{ae} may allow some games to have equilibrium solutions, even if formulation ε did not allow any equilibrium. Additionally, the authors also provide a proof which states that every equilibrium of ε is an equilibrium of ε^{ae}.

In order to transform the latter bi-level problem into a mathematically tractable form, Prob. 2 can be reformulated into a mathematical problem with equilibrium constraints (MPEC), which is described in the subsequent section.

2.2.2. All equilibrium MPEC reformulation

Assuming that a follower *k* problem (PF_k) is convex, i.e. *z* and *m* are respectively convex functions and concave functions in *w*, then for any solution (w_k, ν_k) of the following Karush–Kuhn–Tucker (KKT) optimality conditions, w_k is a global optimal solution of (PF_k). Note that KKT conditions are equivalent to the parametric nonlinear complementarity problem (NCP) (Leyffer and Munson, 2010; Kulkarni and Shanbhag, 2014):

$$\begin{aligned} & \nabla_{w_k} z_k(x_k, w_k, x_{-k}) - \nabla_{w_k} m_k(x_k, w_k, x_{-k}) \nu_k \geq 0 \perp w_k \geq 0 \\ & m_k(x_k, w_k, x_{-k}) \geq 0 \perp \nu_k \geq 0 \\ & k \in L \end{aligned} \tag{Prob. 3}$$

In Prob. 3, ν_k is Lagrange multipliers associated to constraints of the follower $m(x_k, w_k, x_{-k})$. This convexity of the follower problem will be fulfilled for each of the MLSFG and SLMFG formulations of our EIP design problems (cf. Prob. 10–Prob. 14). Indeed in our case the objective function and the constraints of the respective followers are actually linear, thus convex and concave on the variables controlled by the follower. Though, followers' problems may have non-convex terms on the leaders' variables, but they do not affect the non-convexity since they are seen as parameters in the followers' problems.

By substituting follower's problem in each leader problem, the all equilibrium bilevel MLSFG described in Prob. 2 is transformed into the following MPEC for each leader (Prob. 4):

$$\begin{aligned} \min_{\substack{x_i \geq 0 \\ w_i \\ \nu_i}} \quad & f_i(x_i, w_i, x_{-i}) \\ s.t. \quad & \begin{cases} g_i(x_i, w_i, x_{-i}) \geq 0 \\ \nabla_{w_k} z_k(x_k, w_k, x_{-k}) - \nabla_{w_k} m_k(x_k, w_k, x_{-k}) \nu_k \geq 0 \perp w_k \geq 0, \quad \forall k \in L \\ m_k(x_k, w_k, x_{-k}) \geq 0 \perp \nu_k \geq 0, \quad \forall k \in L \end{cases} \end{aligned} \tag{Prob. 4}$$

Note that, depending of the values of coefficients $Cmax^{in/out}$ (see Section 4), the classical qualification conditions may not be fulfilled and thus Prob. 2 and Prob. 4 would not be equivalent. Nevertheless, in all cases, in order to be able to compute through existing theory (Kulkarni and Shanbhag, 2014) and algorithms (Leyffer and Munson, 2010) we systematically replace the followers' problems by their KKT counterpart.

In Prob. 4 it can be seen, that each variable of the follower is duplicated for each leader (even multipliers), in a way consistent with the bilevel ε^{ae} formulation. Then, each leader is now constrained by the KKT conditions of the follower regarding both his own conjecture as other leaders' conjectures. In other words, leaders now control both their own variables, and their own conjectures about follower's response (multipliers included), while they are parameterized by other leaders' variables and their conjectures about follower's response.

Note that Prob. 4 $\forall i \in L$ constitutes a so-called MOPEC (multiple optimization problems with equilibrium constraints). The MLSFG in this form is indeed in a more convenient form in order to solve it. Solution methodologies are explained after introducing the SLMFG formulation.

2.3. Single-leader multi-follower game formulation

The SLMFG formulation is analogue to the formulation featured in Prob. 1, by setting $nl = 1$ and by letting nf be the number of followers, and denote by $F = \{1, \ldots, nf\}$ the index set of followers. Let w_j, $j \in F$ be the decision variables of follower j and w_{-j} the decision variables of other followers. The bilevel SLMFG formulation is then the following:

$$\begin{aligned}
&\min_{\substack{x \geq 0 \\ w}} \quad f(x, w) \\
&\text{subject to} \begin{cases} g(x, w) \geq 0 \\ \forall j \in F, w_j \quad \text{solves}: \\ \left.\begin{array}{l} \min\limits_{w_j \geq 0} \quad z_j(x, w_j, w_{-j}) \\ s.t. \left\{ m_j(x, w_j, w_{-j}) \geq 0 \right. \end{array}\right\} (PF_j) \end{cases}
\end{aligned} \qquad \text{(Prob. 5)}$$

In Prob. 5, followers play a Nash game among them, given the equilibrium of the leader. It is important to note that even if MLSFG and SLMFG are both MLFG the nature of the problem to be solved changes drastically. On the first hand, for SLMFG ε and ε^{ae} formulations discussion is not applicable, since there is only one shared leader among followers, thus there exists only one conjecture of followers' equilibriums. On the other hand, the informal description of the game is the following: for every vector of x the followers calculate their equilibria. Then, the leader selects among the obtained solutions, the couple (x, w) whichever minimizes f.

As the SLMFG is indifferent of ε and ε^{ae} formulations, the MPEC transformation of the bilevel problem is given by Prob. 6, where each follower's KKT is now part of the leader optimization problem:

$$\begin{aligned}
&\min_{\substack{x \geq 0 \\ w_j \\ \nu_j}} \quad f_i(x, w_j) \\
&\text{s.t.} \begin{cases} g(x, w_j) \geq 0 \\ \nabla_{w_j} z_j(x, w_j, w_{-j}) - \nabla_{w_j} m_j(x, w_j, w_{-j}) \nu_j \geq 0 \perp w_j \geq 0, \quad \forall j \in F \\ m_j(x, w_j, w_{-j}) \geq 0 \perp \nu_j \geq 0, \quad \forall j \in F \end{cases}
\end{aligned} \qquad \text{(Prob. 6)}$$

Remark that Prob. 6 constitutes a sole MPEC by contrast to the MOPEC formed by the MLSFG formulation. Consequently, MLSFG are harder to solve than SLMFG. However, both formulations share solution methodologies, which are discussed in detail in the following subsection. Let us also observe that the transformation of Prob. 5 into Prob. 6 is valid under the condition that for any j the functions z_j and m_j are respectively convex and concave in terms of w_j and some qualification conditions hold true.

2.4. Solution methodologies

As discussed earlier, both MLSFG and SLMFG are solved in a very similar way. Consequently, in this section the solution methodologies are explained explicitly for the MLSFG all equilibrium MPEC formulation (cf. Prob. 4). The equivalent resultant problem for the SLMFG is presented as well, given the analogies between the former and the latter.

Generally, one computationally attractive way to solve MLFG consists in replacing each leader MPEC by its strong stationarity conditions and concatenate all resultant KKT conditions (Leyffer and Munson, 2010; Facchinei and Pang, 2007). It is important to note that the resultant optimization problems are always non-convex due to the presence of complementarity constraints. Then, by using this method in reality strong stationarity points are obtained for each optimization problem. By itself, the problem derived with this method is an NCP (Prob. 7), using the MPEC in Prob. 4. For the sake of simplicity, follower's inequality KKT constraints are grouped as follows:

$$\begin{aligned}
&r_i = (w_i, \nu_i) \\
&s_i(x_i, r_i, x_{-i}) = \begin{pmatrix} \nabla_{w_i} z_i(x_i, w_i, x_{-i}) - \nabla_{w_i} m_i(x_i, w_i, x_{-i}) \nu_i \\ m_i(x_i, w_i, x_{-i}) \end{pmatrix} \\
&i \in L
\end{aligned} \qquad (1)$$

$$\begin{aligned}
&\nabla_{x_i} f_i(x_i, w_i, x_{-i}) - \nabla_{x_i} g_i(x_i, w_i, x_{-i}) \mu_i - \sum_{k \in L} \nabla_{x_i} s_k(x_i, r_k, x_{-i}) \xi_k \geq 0 \perp x_i \geq 0, \quad \forall i \in L \\
&\nabla_{r_i} f_i(x_i, w_i, x_{-i}) - \nabla_{r_i} g_i(x_i, w_i, x_{-i}) \mu_i - \sum_{k \in L} \nabla_{r_i} s_k(x_i, r_k, x_{-i}) \xi_k \geq 0 \perp r_i \geq 0, \quad \forall i \in L \\
&g_i(x_i, w_i, x_{-i}) \geq 0 \perp \mu_i \geq 0, \quad \forall i \in L \\
&s_k(x_i, r_k, x_{-i}) \geq 0 \perp \xi_k \geq 0, \quad \forall k \in L \\
&s_k(x_i, r_k, x_{-i}) \geq 0 \perp r_k \geq 0, \quad \forall k \in L
\end{aligned} \qquad \text{(Prob. 7)}$$

where $\nabla_{x_i} \; g_i(x_i, w_i, x_{-i})$ and $\nabla_{x_i} \; s_k(x_i, r_k, x_{-i})$ stand respectively for the Jacobian matrix of vector-valued functions g_i and s_k.

Note that Prob. 7 is not a squared NCP, since each r_k is matched with two orthogonality constraints. Therefore, this formulation is very hard to solve (and even more for large-scale problems) by using standard NCP solvers (i.e. PATH (Dirkse and Ferris, 1996)) since constraints violate any classical constraint qualification due to the presence of complementarity conditions (Leyffer and Munson, 2010).

However, the NCP formulation illustrated in Prob. 7 can be used to derive NLP formulations of a MLFG. A very interesting alternative which exploits the capacity of modern NLP solvers is the so-called penalty formulation (Biegler, 2010). This formulation consists in moving the complementarity constraints to the objective function, which is minimized. The latter is very convenient for the MLSFG, since it do not exhibit a typical NLP formulation, i.e. no objective function. Hence, the remaining constraints are well behaved. The formulation for the MLSFG is illustrated next (Prob. 8), after introducing slacks π_i, η_i, τ_i, φ_i to inequalities:

$$\begin{aligned} \min_{\substack{x, r, \\ \mu, \xi, \\ \pi, \eta, \\ \tau, \varphi}} \quad & C_{pen} = \sum_{i' \in L} \left[x_{i'}^T \pi_{i'} + \mu_{i'}^T \tau_{i'} + w_{i'}^T \eta_{i'} + \varphi_{i'}^T \xi_{i'} + \varphi_{i'}^T r_{i'} \right] \\ s.t. \quad & \begin{cases} \nabla_{x_i} f_i(x_i, w_i, x_{-i}) - \nabla_{x_i} g_i(x_i, w_i, x_{-i})\mu_i - \sum_{k \in L} \nabla_{x_i} s_k(x_i, r_k, x_{-i})\xi_k = \pi_i, & \forall i \in L \\ \nabla_{r_i} f_i(x_i, w_i, x_{-i}) - \nabla_{r_i} g_i(x_i, w_i, x_{-i})\mu_i - \sum_{k \in L} \nabla_{r_i} s_k(x_i, r_k, x_{-i})\xi_k = \eta_i, & \forall i \in L \\ g_i(x_i, w_i, x_{-i}) = \tau_i, & \forall i \in L \\ s_k(x_i, r_k, x_{-i}) = \varphi_k, & \forall k \in L \\ x_i \geq 0, r_i \geq 0, \mu_i \geq 0, \xi_i \geq 0, \pi_i \geq 0, \eta_i \geq 0, \tau_i \geq 0, \varphi_i \geq 0, & \forall i \in L \end{cases} \end{aligned} \tag{Prob. 8}$$

The above formulation is in fact one of the several formulations to solve general MPEC problems (cf. Biegler, 2010) for all possible formulations and it is the most adequate to solve MLFG problems and MPECs in general (Biegler, 2010). In addition, Leyffer and Munson (2010) proved that if $C_{pen} = 0$ and if all variables describe a local solution of the minimization problem, then the solution is a strong stationarity point of the MLFG. By moving complementarities to the objective function, most difficulties of the NCP formulation are overcome including the non-square nature of Prob. 7. The analogous formulation for the SLMFG is described in Prob. 9, where $\rho > 0$ corresponds to a penalization parameter:

$$\begin{aligned} \min_{\substack{x, r, \\ \tau, \varphi}} \quad & C' = f(x, w) + \rho \sum_{j \in F} \varphi_j^T r_j \\ s.t. \quad & \begin{cases} g(x, w) = \tau \\ s_j(x, r_j, r_{-j}) = \varphi_j, & \forall j \in F \\ \tau \geq 0 \\ x \geq 0 \\ r_j \geq 0, \varphi_j \geq 0, & \forall j \in F \end{cases} \end{aligned} \tag{Prob. 9}$$

In this work, both NCP and NLP solution methods were tested. However, the NLP formulation is preferred for the reasons stated above. All problems were modelled in GAMS® (Brooke et al., 1998) 24.4.2 and transformed into Prob. 7 through the extended mathematical programming framework (EMP). The framework uses the solver JAMS to reformulate Nash games (in MPEC form) into NCPs. Evidently, it is the modeller task to transform the original MLFG into his MPEC formulation. Then, it is the modeller choice to solve it through Prob. 7 or Prob. 8/Prob. 9 formulation. In the former case, the solver employed has to be capable of solving NCP, e.g. PATH (Dirkse and Ferris, 1996) and in the latter a standard NLP solver is required. In this work, a combination of CONOPT, IPOPTH (Wächter and Biegler, 2002) and BARON (Tawarmalani and Sahinidis, 2005) (if one solver fails to find a solution, then the other is called) was used. In the context of a penalization scheme like the one in Prob. 8, a global solver like BARON is very useful to find the solution where $C_{pen} = 0$. Moreover, recent work (Zhang and Sahinidis, Globa) demonstrated the usefulness of BARON in general MPCC problems, using recent versions of it. All results reported in this work are those corresponding to the solution of Prob. 8/Prob. 9 formulation.

In the following section, the EIP specific model is introduced, with their specific MLFG formulations and results of each specific case study.

3. EIP problem statement, case studies and results

Water integration in EIP is modelled as an industrial water network (IWN) allocation problem, according to numerous previous works (Boix et al., 2010; Ramos et al., 2014; Pang et al., 2005; Kulkarni and Shanbhag, 2014). Indeed, the way to model a IWN allocation problem is based on the concept of superstructure (Yeomans and Grossmann, 1999; Biegler et al., 1997). From a given number of regeneration units and processes, all possible connections between them may exist, except recycling to the same unit. This constraint forbids self-recycles on process and regeneration units, although the latter is often relevant in some chemical processes. For each water flowrate using process, input water may be freshwater, output water from other processes and/or regenerated water. Indeed, output water from a process may be directly discharged, distributed to another process and/or to regeneration units. For the sake of simplicity and generalization, the problem is built as a set of black boxes. In this kind of approach, physical or chemical phenomena occurring inside each process is not taken into account. In addition, each process has a contaminant load over the input flowrate of water. As aforementioned, only one contaminant is considered in the presented EIP. A general view of the superstructure is given in Fig. 4.

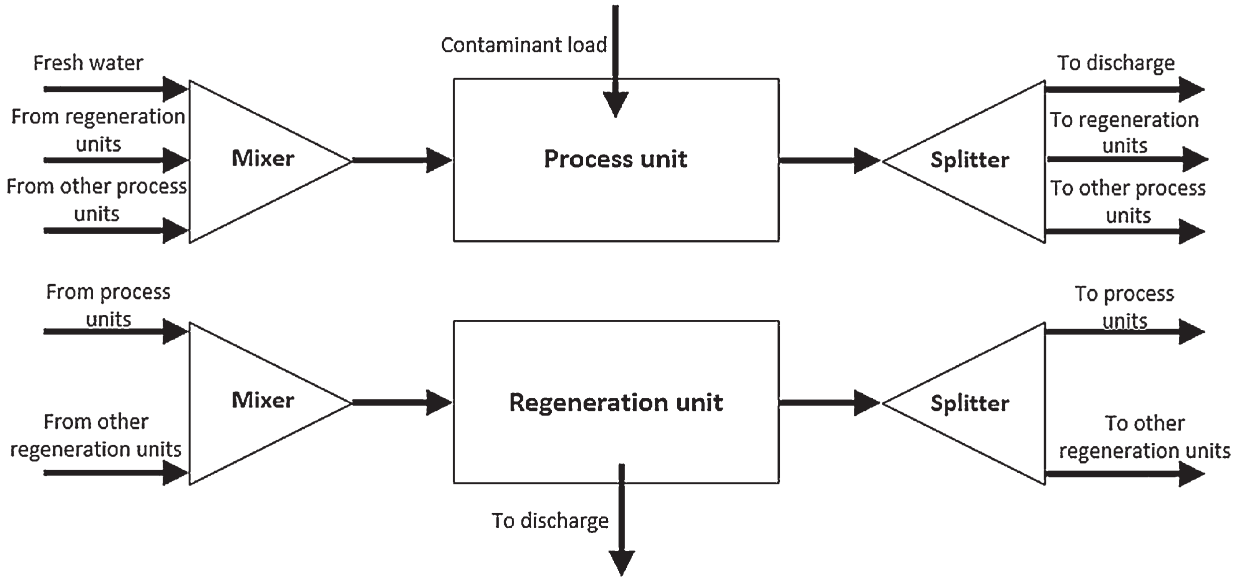

Fig. 4. General view of the superstructure for IWN allocation problem (modified from Boix et al., 2012).

Mathematically speaking, let *np* denote the given number of processes per enterprise, $P = \{1, 2, \ldots, np\}$ denote the index set of processes, and let *nep* denote the given number of enterprises/plants in the EIP, $EP = \{1, 2, \ldots, nep\}$ denote the index set of enterprises/plants; let *nr* denote the total number of regeneration units, $R = \{1, \ldots, nr\}$ denote the index set of regeneration units. Each process $p \in P$ of each enterprise $ep \in EP$ has a given contaminant load, denoted by $M_{ep,p}$, a given maximum concentration of contaminant allowed either in the inlet as in the outlet, denoted by $Cmax^{in}_{ep,p}$, $Cmax^{out}_{ep,p}$ respectively. It is important to highlight that contaminant partial flows are neglected, since their magnitude is considerably lower in comparison to water flows. Therefore, it is assumed that the total flow between processes is equivalent to only water flowrate. Moreover, it is assumed that processes will only consume the exact amount of water needed to satisfy concentration constraints. Consequently, processes water outlet will have a concentration equivalent to $Cmax^{out}_{ep,p}$ (cf. Bagajewicz and Faria, 2009) for detailed explanation. Equivalently, each regeneration unit $r \in R$ has a given output contaminant concentration, denoted by C^{out}_{r}. In terms of variables, each process of each enterprise $p \in P$, $ep \in EP$ sends water to process $p' \in P$ of enterprise $ep' \in EP$, $\{ep', p'\} \neq \{ep, p\}$, taken into account by variable $Fpart_{ep,p,ep',p'}$, receives water, denoted by variable $Fpart_{ep',p',ep,p}$ and has an inlet flow of freshwater, denoted by $Fw_{ep,p}$. In addition, each process may send polluted water to regeneration unit $r \in R$ or receive low contaminant concentration water by the latter, denoted by $Fproreg_{ep,p,r}$, $Fregpro_{r,ep,p}$ respectively, or may send water directly to the discharge, denoted by $Fdis_{ep,p}$.

Finally, it is to be noted that the original model (e.g. Bagajewicz and Faria, 2009; Boix et al., 2012; Ramos et al., 2014) was formulated as a mixed-integer linear programme (MILP), since it takes into account minimum allowable flowrate between processes and/or regeneration units (namely, the minimum allowed water flowrate was fixed at 2 T/h in Boix et al. (2012)). Nevertheless, in a MLFG formulation discrete variables are rather impossible to handle (at least for now). In consequence, in the present article minimum flowrate *minf* is handled by an elimination algorithm which is explained afterwards.

3.1. Model without regeneration units formulation

Given the aforementioned notation, the model without regeneration units presented by Ramos et al. (2014) for the IWN in EIP is presented below:

- Water mass balance around a process unit $p \in P$ of an enterprise $ep \in EP$:

$$Fw_{ep,p} + \sum_{ep' \in EP} \sum_{p' \in P} Fpart_{ep',p',ep,p} = \sum_{ep' \in EP} \sum_{p' \in P} Fpart_{ep,p,ep',p'} + Fdis_{ep,p} \quad \{ep, p\} \neq \{ep', p'\} \tag{2}$$

- Contaminant mass balance around a process unit $p \in P$ of an enterprise $ep \in EP$:

$$M_{ep,p} + \sum_{ep' \in EP} \sum_{p' \in P} Cmax^{out}_{ep',p'} Fpart_{ep',p',ep,p} = Cmax^{out}_{ep,p} \left(\sum_{ep' \in EP} \sum_{p' \in P} Fpart_{ep,p,ep',p'} + Fdis_{ep,p} \right) \quad \{ep, p\} \neq \{ep', p'\} \tag{3}$$

- Inlet/outlet concentration constraints for a process unit $p \in P$ of an enterprise $ep \in EP$:

$$\sum_{ep' \in EP} \sum_{p' \in P} Cmax^{out}_{ep',p'} Fpart_{ep',p',ep,p} \leq Cmax^{in}_{ep,p} \left(Fw_{ep,p} + \sum_{ep' \in EP} \sum_{p' \in P} Fpart_{ep',p',ep,p} \right) \quad \{ep, p\} \neq \{ep', p'\} \tag{4}$$

- Freshwater positivity for a process unit $p \in P$ of an enterprise $ep \in EP$:

$$Fw_{ep,p} \geq 0 \tag{5}$$

- Flow between processes positivity going from a process unit $p \in P$ of an enterprise $ep \in EP$ to a process $p' \in P$ of an enterprise $ep' \in EP$, $\{ep', p'\} \neq \{ep, p\}$:

$$Fpart_{ep,p,ep',p'} \geq 0 \tag{6}$$

- Discharge flow positivity for a process unit $p \in P$ of an enterprise $ep \in EP$:

$$Fdis_{ep,p} \geq 0 \tag{7}$$

From the aforementioned equations, some variables may be eliminated in order to produce a more succinct model with less variables but equivalent. Indeed, by combining Eqs. (2) and (3) we obtain:

$$M_{ep,p} + \sum_{ep' \in EP} \sum_{p' \in P} Cmax^{out}_{ep',p'} Fpart_{ep',p',ep,p} = Cmax^{out}_{ep,p} \left(Fw_{ep,p} + \sum_{ep' \in EP} \sum_{p' \in P} Fpart_{ep',p',ep,p} \right) \quad \forall ep \in EP, p \in P \quad \{ep, p\} \neq \{ep', p'\} \tag{8}$$

As $Fdis_{ep,p}$ is now eliminated from the model, his positivity constraint is now expressed as follows:

$$Fw_{ep,p} + \sum_{ep' \in EP} \sum_{p' \in P} Fpart_{ep',p',ep,p} \geq \sum_{ep' \in EP} \sum_{p' \in P} Fpart_{ep,p,ep',p'} \quad \forall ep \in EP, p \in P \quad \{ep, p\} \neq \{ep', p'\} \tag{9}$$

From the aforementioned model, MLSFG and SLMFG problems are formulated, depending on the structures shown in Figs. 3 and 2, respectively. For both cases, an enterprise $ep \in EP$ aims to minimize his annualized operating cost, defined by:

$$C^{tot}_{ep}(Fpart, Fpart, Fw) = AWH \left[\alpha \sum_{p \in P} Fw_{ep,p} + \beta \sum_{p \in P} \left(Fw + \sum_{ep' \in EP} \sum_{p' \in P} Fpart_{ep',p',ep,p} - \sum_{ep' \in EP} \sum_{p' \in P} Fpart_{ep,p,ep',p'} \right) \right.$$

$$\left. + \delta \sum_{p \in P} \sum_{\substack{p' \in P \\ p \neq p'}} Fpart_{ep,p,ep,p'} + \frac{\delta}{2} \sum_{\substack{ep' \in EP \\ ep' \neq ep}} \sum_{p' \in P} \sum_{p \in P} \left(Fpart_{ep,p,ep',p'} + Fpart_{ep',p',ep,p} \right) \right], \tag{10}$$

where α stands for the purchase price of freshwater, β for the cost associated to polluted water discharge and δ for the cost of pumping polluted water from one process to another. Indeed, each enterprise pays the cost of pumping water both to a process and from a process. Remark that each enterprise pays the totality of the cost associated with water pumping between their processes, and regarding water shared with and from other enterprises the cost is shared between enterprises instead (i.e. $\delta/2$). On the other hand, the EIP authority aims to minimize total freshwater consumption in the EIP.

In the MLSFG problem, enterprises act as leaders and the EIP authority as the common follower. In order to maintain the same notation as in Section 3, we define:

$$\begin{aligned} Fw &= (Fw_{ep,p} : 1 \leq ep \leq nep, 1 \leq p \leq np) \\ Fpart_{ep} &= (Fpart_{ep,p,ep',p'} : 1 \leq ep' \leq nep, 1 \leq p, p' \leq np, \{ep, p\} \neq \{ep', p'\}) \end{aligned} \tag{11}$$

Formally, each enterprise's $ep \in EP$ optimization problem is the following:

$$\begin{aligned} &\min_{\substack{Fpart_{ep} \\ Fw}} \quad C^{tot}_{ep}(Fpart_{ep}, Fpart_{-ep}, Fw) \\ &s.t. \begin{cases} Fpart_{ep} \geq 0 \\ Fw \ \text{ solves :} \\ \min_{Fw} \ \sum_{ep \in EP} \sum_{p \in P} Fw_{ep,p} \\ s.t. \left\{ \text{Eq. 4} - \text{Eq. 5}, \ \text{Eq. 8} - \text{Eq. 9} \right. \end{cases} \end{aligned} \tag{Prob. 10}$$

As it can be seen from Prob. 10, each enterprise controls the flows from each one of its processes to all other processes (included those to other enterprises), while his problem is parameterized by the same respective variables of other enterprises and the freshwater flow to its processes, controlled by the follower.

On the other hand, on the SLMFG problem, the common leader is the EIP authority and the followers are the enterprises. Using the above notation, the formal definition of the problem is the following:

$$\min_{\substack{Fw \\ Fpart}} \sum_{ep \in EP} \sum_{p \in P} Fw_{ep,p}$$
$$s.t. \begin{cases} Fw \geq 0 \\ Fpart_{ep} \ \text{ solves } \ \forall ep \in EP: \\ \min\limits_{Fpart_{ep}} \ C^{tot}_{ep}(Fpart_{ep}, Fpart_{-ep}, Fw) \\ s.t. \left\{ \text{Eq. 4, Eq. 6, Eq. 8} - \text{Eq. 9} \right. \end{cases} \tag{Prob. 11}$$

In this case, the game consists in: between the different possible Nash equilibrium for the Nash Game, defined by the family of enterprises' problems, parameterized by the vector *Fw*, the leader (regulator) chooses the equilibrium for which the total freshwater consumption in the EIP in minimized.

Actually the MLSFG formulation (Prob. 10) can be further simplified: as it can be noted, a direct expression for freshwater flowrate can be derived from Eq. (8). By deriving the latter and by replacing in Prob. 10, the follower problem disappears to produce an equivalent GNEP between enterprises (Eqs. (12)–(14)), thus dropping the bilevel structure.

$$\sum_{ep' \in EP} \sum_{p' \in P} Cmax^{out}_{ep',p'} Fpart_{ep',p',ep,p} \leq \frac{Cmax^{in}_{ep,p}}{Cmax^{out}_{ep,p}} \left(M_{ep,p} + \sum_{ep' \in EP} \sum_{p' \in P} Cmax^{out}_{ep',p'} Fpart_{ep',p',ep,p} \right) \quad \forall ep \in EP, p \in P, \{ep, p\} \neq \{ep', p'\} \tag{12}$$

$$M_{ep,p} + \sum_{ep' \in EP} \sum_{p' \in P} Cmax^{out}_{ep',p'} Fpart_{ep',p',ep,p} \geq Cmax^{out}_{ep,p} \sum_{ep' \in EP} \sum_{p' \in P} Fpart_{ep,p,ep',p'} \quad \forall ep \in EP, p \in P, \{ep, p\} \neq \{ep', p'\} \tag{13}$$

$$M_{ep,p} + \sum_{ep' \in EP} \sum_{p' \in P} Cmax^{out}_{ep',p'} Fpart_{ep',p',ep,p} - Cmax^{out}_{ep,p} \sum_{ep' \in EP} \sum_{p' \in P} Fpart_{ep',p',ep,p} \geq 0 \quad \forall ep \in EP, p \in P, \{ep, p\} \neq \{ep', p'\} \tag{14}$$

Then, each enterprise's $ep \in EP$ optimization problem is defined as follows:

$$\min_{Fpart_{ep}} C^{tot}_{ep}(Fpart_{ep}, Fpart_{-ep})$$
$$s.t. \begin{cases} \text{Eq. 6} \\ \text{Eq. 12} - \text{Eq. 14} \end{cases} \tag{Prob. 12}$$

The formulation illustrated in Prob. 12 will be used for the case of EIP without regeneration units. Nevertheless, for the case of SLMFG the problem cannot be simplified as stated above, since the nature of the problem does not allow it (i.e. minimization of freshwater consumption in the upper level). Summarizing, the corresponding formulations used in the present work are Prob. 11 and Prob. 12, for the case without regeneration units.

3.1.1. Low-flowrate elimination algorithm

Another important point is the replacement of discrete decisions in the MLFG framework. Indeed with available optimization methods and solvers for MINLP problems, it is not reasonable to be thinking of considering binary or integer variables. Thus as explained at beginning of Section 4, we initially consider all possible connections between processes, and between processes and regeneration units through the variables *Fpart*, *Fproreg* and *Fregpro* respectively.

Note that any connection is represented by two variables since we consider only non-negative flow variables. Then, we apply a finite sequence of steps, each step being composed of first the resolution of the MLSFG/SLMFG problem in his NLP formulation (Prob. 8/Prob. 9), second, an elimination procedure that aims to force to zero the flow of any oriented connection for which step 1 gave a flow lower that a minimum fixed bound min*f*. This is indeed modelled by big-M constraints and binary variables in the former classical water integration (Ramos et al., 2014; Bagajewicz and Faria, 2009) model. In this work, we developed an a posteriori algorithm to add bounds to existing flows and to eliminate low flows. Indeed, the MLFG is solved several times until all flows are equal or superior to min*f*. The algorithm is described in detail next, using as example $Fpart_{ep,p,ep',p'}$ (all other flows are handled simultaneously and equivalently):

1) The initial MLFG is solved to optimality.
2) For all $ep, ep' \in EP$, $p, p' \in P$, $\{ep, p\} \neq \{ep', p'\}$:
   a. If $Fpart_{ep,p,ep',p'} \geq \frac{3}{4} \min f$, then a lower bound of the flow is imposed that is the constraint $Fpart_{ep,p,ep',p'} \geq \min f$ is added to the model.
   b. If $Fpart_{ep,p,ep',p'} < \frac{3}{4} \min f$, then the flow is fixed $Fpart_{ep,p,ep',p'} = 0$
   c. Else, if all flows $Fpart_{ep,p,ep',p'} \geq \min f$, then the problem has converged and no further treatment is required.
3) The bound-modified MLFG problem is tried to be solved to optimality:
   a. If optimality is achieved, then go to 2).
   b. Else, try solving to optimality with a different solver.
      i. If optimality is achieved, then go to 2).
      ii. Else, restore initial bounds of the variables of the process whose constraint/s are infeasible. Go to 3).

In the aforementioned way, low-flowrates are systematically eliminated. It is important to note that in our numerical experience the algorithm almost never failed by bounding critical flows thus driving to infeasible models. However, it is evident that the solution obtained

Table 2
Case study parameters (Olesen and Polley, 1996).

Enterprise	Process	$C_{\max}$(ppm)	$C_{\max}$(ppm)	$M_{ep,p}(g/h)$
1	1	0	100	2000
	2	50	80	2000
	3	50	100	5000
	4	80	800	30,000
	5	400	800	4000
2	1	0	100	2000
	2	50	80	2000
	3	80	400	5000
	4	100	800	30,000
	5	400	1000	4000
3	1	0	100	2000
	2	25	50	2000
	3	25	125	5000
	4	50	800	30,000
	5	100	150	15,000

Table 3
Associated costs.

Parameter	Value ($/tonne)
α	0.13
β	0.22
δ	2e-2

does not assure in any way neither local nor global optimality in terms only of discrete decisions. Nevertheless, it represents an efficient way to deal with the latter, given the natural complexity of the problem.

3.1.2. Case study, results and discussion

All problems were initialized with the trivial feasible solution where the flows between enterprises do not exist, i.e. $Fpart_{ep,p,ep',p'} = 0$, $\forall\, ep, ep' \in EP, p, p' \in P, \{ep, p\} \neq \{ep', p'\}$, and therefore, processes are only fed with freshwater. It is important to note that this solution represents a feasible solution (at least for the concentration constraints) that is indeed far from being optimal solution. It is then important to be particularly careful with the initialization of the problem, due to its non-convex and nonlinear nature.

The case study consists on an EIP made up of 3 enterprises each one with 5 processes. In fact, it consists on a hypothetic literature example originally developed by Olesen and Polley (1996) and then modified by different authors (Boix et al., 2012; Chew et al., 2009) in order to use it in an EIP context. Parameters of this case study are given in Table 2.

Additionally, prices are shown in Table 3. Freshwater and discharged water cost is extracted from Chew et al. (2008) (which is assumed to include pumping) and the approximated cost of pumping water between processes is calculated by simulating the energy consumption of pumping 1 T/h of water in Aspen Plus® with a Δ Pressure of 3 bar. The minimum flowrate allowed is min$f$ = 2 T/h and it is assumed that the EIP operates AWH = 8000 hours/year. As mentioned earlier, results obtained are mainly compared to both the results obtained with classic MOO (the original MILP model cf. Boix et al., 2012), and solved through GP with weight factors = 1 for all objective functions and minimizing the distance to the ideal solution, cf. Ramos et al. (2014) and the case where all enterprises operate by themselves, i.e. no EIP exists. Results obtained consist on MLSFG and SLMFG solutions and are illustrated as follows: first, the case where there is no EIP (i.e. each enterprise by itself) in Table 4 and EIP results in Table 5.

Optimization problems Prob. 8–Prob. 12 and Prob. 9–Prob. 11 respectively associated to MLSFG and SLMFG have respectively, as reported by GAMS, 2164 and 522 continuous variables, and 1401 and 261 constraints. Solution times were 5.3 CPUs and 25.2 CPUs. The latter solution time is due to the addition of low-flow elimination algorithm.

Results shown above underline several important points. In the first place, it is obvious that enterprise 3 is the most water-demanding one, since its production (represented by $M_{ep,p}$) is considerably higher than other enterprises. Consequently, its operating cost is higher. Then, another important aspect is that enterprises naturally consume more freshwater when they operate by themselves (i.e. ~340 tonne/h) that when they operate inside the EIP (i.e. ~314 tonne/h). Also, from the MOO solution it can be seen that enterprises take advantage of exchanges throughout the EIP configuration to minimize their operating cost. Nevertheless, it is to be noted that only enterprises 1 and 2 achieve an operating cost inferior to the case where they operate alone. Indeed, this is exactly the kind of drawback discussed earlier in this work regarding MOO techniques and specifically GP. Under these conditions, it is manifest that enterprise 3 will not be interested into participating in an EIP.

Table 4
Results of each enterprise operating by itself without regeneration units.

Enterprise		1	2	3	Total
Water flowrate (T/h)	Fresh	98.33	54.64	186.67	339.64
	Freshwater + discharge	0.28	0.15	0.52	0.95
Cost (MMUSD/year)	Reused water	0.01	0.01	0.02	0.03
	Total	0.28	0.16	0.54	0.98

Table 5
Summary of results of the EIP without regeneration units.

MOO					
Enterprise		1	2	3	Total
Water flowrate (T/h)	Fresh	88.33	20.00	206.02	314.36
	Shared	76.67	61.04	82.00	219.71
	Freshwater + Discharge	0.18	0.11	0.59	0.88
Cost (MMUSD/year)	Reused water	0.01	0.02	0.02	0.06
	Total	0.20	0.13	0.61	0.94
Nash equilibrium (MLSFG)					
Enterprise		1	2	3	Total
Water flowrate (T/h)	Freshwater (tonne/h)	146.67	33.62	134.06	314.35
	Shared	186.67	84.18	138.73	409.58
	Freshwater + Discharge	0.24	0.13	0.50	0.88
Cost (MMUSD/year)	Reused water	0.02	0.02	0.03	0.07
	Total	0.27	0.15	0.54	0.95
Nash equilibrium (SLMFG)					
Enterprise		1	2	3	Total
Water flowrate (T/h)	Freshwater (tonne/h)	136.59	39.34	138.42	314.35
	Shared	186.67	96.67	140.16	423.49
	Freshwater + Discharge	0.23	0.14	0.52	0.89
Cost (MMUSD/year)	Reused water	0.02	0.02	0.02	0.06
	Total	0.26	0.16	0.54	0.95

Regarding Nash equilibrium solutions, it can be seen that for the MLSFG case all enterprises are satisfied since each enterprise's annual operating cost is inferior to when operating by themselves, even if enterprise 3 has a very low gain. On the other hand, the SLMFG solution satisfies every enterprise but enterprise 3, where the operating cost is equal to the case where it operates alone. Indeed, it is remarkable that regarding freshwater consumption, MLSFG and SLMFG provide different results, which is completely coherent with both formulations. For instance, enterprises have a relative gain of 5.77%, 8.45% and 0.38% respectively in the former formulation, and 9.2%, 5.09% and 0.0%. It is noticeable that sharing water cost is very inferior to freshwater and discharge cost, hence, benefits that can be achieved by sharing water between enterprises is still low. With introduction of regeneration units, the latter cost can be lowered and can favour exchanges between enterprises.

At this point, an important remark has to be made. In a real context, an EIP should be made up of several more enterprises working in symbiosis. Therefore, it is crucial to analyze scaling of the formulation in order to analyze if it can be suited to a real EIP context. For this purpose, we generated and ran a test with 10 enterprises each one with 5 processes maintaining the former three enterprises and adding 7 fictional enterprises, by using similar contaminant charge M and similar $Cmax^{in/out}$ to the original case study in a SLMFG configuration. Resulting test problem consisted of 7483 continuous variables and 3970 constraints. We solved to optimality a single instance of Prob. 8–Prob. 11 (without applying the low-flowrate elimination algorithm) in 16.5 CPUs. The solution obtained contained no more than 0.53% of low-flowrates. Thus, it emphasize that it is still feasible to run real-world large-scale of the formulation presented in this work in decent CPU time.

3.2. Model with regeneration units formulation

The model with regeneration units has the same basis of the aforementioned model. It is assumed that all regeneration units are shared and that the EIP authority is concerned with all decisions involved with them since on an EIP context the more convenient is to share all resources. Indeed, early results with these kinds of considerations were not consistent with EIP philosophies. Therefore, only shared regeneration units are considered, i.e. owned by the EIP.

Model constraints are as follows, consistent with the formulation mentioned earlier in this section:

- Water mass balance around a process unit $p \in P$ of an enterprise $ep \in EP$:

$$Fw_{ep,p} + \sum_{ep' \in EP} \sum_{p' \in P} Fpart_{ep',p',ep,p} + \sum_{r \in R} Fregpro_{r,ep,p} = \sum_{ep' \in EP} \sum_{p' \in P} Fpart_{ep,p,ep',p'} + \sum_{r \in R} Fregpro_{r,ep,p} + Fdis_{ep,p} \quad \{ep, p\} \neq \{ep', p'\} \tag{15}$$

- Contaminant mass balance around a process unit $p \in P$ of an enterprise $ep \in EP$:

$$M_{ep,p} + \sum_{ep' \in EP} \sum_{p' \in P} Cmax^{out}_{ep',p'} Fpart_{ep',p',ep,p} + \sum_{r \in R} C^{out}_r Fregpro_{r,ep,p}$$
$$= Cmax^{out}_{ep,p} \left(\sum_{ep' \in EP} \sum_{p' \in P} Fpart_{ep,p,ep',p'} + \sum_{r \in R} Fregpro_{r,ep,p} + Fdis_{ep,p} \right) \quad \{ep, p\} \neq \{ep', p'\} \tag{16}$$

- Inlet/outlet concentration constraints for a process unit $p \in P$ of an enterprise $ep \in EP$:

$$\sum_{ep' \in EP} \sum_{p' \in P} Cmax^{out}_{ep',p'} Fpart_{ep',p',ep,p} + \sum_{r \in R} C^{out}_{r} Fregpro_{r,ep,p} \leq Cmax^{in}_{ep,p} \left(Fw_{ep,p} + \sum_{ep' \in EP} \sum_{p' \in P} Fpart_{ep',p',ep,p} + \sum_{r \in R} Fregpro_{r,ep,p} \right) \quad \{ep, p\} \neq \{ep', p'\} \tag{17}$$

- Contaminant concentration constraints for regeneration unit $r \in R$:

$$\sum_{ep \in EP} \sum_{p \in P} Cmax^{out}_{ep,p} Fproreg_{ep,p,r} \geq C^{out}_{r} \sum_{ep \in EP} \sum_{p \in P} Fregpro_{r,ep,p} \tag{18}$$

- Mass balance around a regeneration unit $r \in R$ (water and contaminant losses are neglected):

$$\sum_{ep \in EP} \sum_{p \in P} Fproreg_{ep,p,r} = \sum_{ep \in EP} \sum_{p \in P} Fregpro_{r,ep,p} \tag{19}$$

- Flow between processes and regeneration unit positivity going from a process unit $p \in P$ of an enterprise $ep \in EP$ to a regeneration unit $r \in R$:

$$Fproreg_{ep,p,r} \geq 0 \tag{20}$$

- Flow between regeneration unit to a process unit $p \in P$ of an enterprise $ep \in EP$ from a regeneration unit $r \in R$:

$$Fregpro_{r,ep,p} \geq 0 \tag{21}$$

- In the same way as is the model without regeneration units, combining Eq. (15) with Eq. (16) leads to:

$$M_{ep,p} + \sum_{ep' \in EP} \sum_{p' \in P} Cmax^{out}_{ep',p'} Fpart_{ep',p',ep,p} + \sum_{r \in R} C^{out}_{r} Fregpro_{r,ep,p} = Cmax^{out}_{ep,p} \left(Fw_{ep,p} + \sum_{ep' \in EP} \sum_{p' \in P} Fpart_{ep',p',ep,p} + \sum_{r \in R} Fregpro_{r,ep,p} \right) \quad \{ep, p\} \neq \{ep', p'\} \tag{22}$$

- $Fdis_{ep,p}$ positivity for a process unit $p \in P$ of an enterprise $ep \in EP$:

$$Fw_{ep,p} + \sum_{ep' \in EP} \sum_{p' \in P} Fpart_{ep',p',ep,p} + \sum_{r \in R} Fregpro_{r,ep,p} \geq \sum_{ep' \in EP} \sum_{p' \in P} Fpart_{ep,p,ep',p'} + \sum_{r \in R} Fproreg_{ep,p,r} \quad \{ep, p\} \neq \{ep', p'\} \tag{23}$$

Given these simplifications, the total annual operating cost of each enterprise $ep \in EP$ is redefined as follows:

$$C^{tot}_{ep}(Fpart, Fw, Fproreg, Fregpro) = AWH \left[\alpha \sum_{p \in P} Fw_{ep,p} + \beta \sum_{p \in P} \left(\begin{array}{l} Fw_{ep,p} + \sum_{ep' \in EP} \sum_{p' \in P} Fpart_{ep',p',ep,p} + \sum_{r \in R} Fregpro_{r,ep,p} - \\ \sum_{ep' \in EP} \sum_{p' \in P} Fpart_{ep,p,ep',p'} + \sum_{r \in R} Fregpro_{r,ep,p} \end{array} \right) \delta \left(\begin{array}{l} \sum_{p \in P} \sum_{\substack{p' \in P \\ p \neq p'}} Fpart_{ep,p,ep,p'} + \\ \sum_{r \in R} \sum_{p \in P} \left(Fproreg_{ep,p,r} + Fregpro_{r,ep,p} \right) \end{array} \right) + \frac{\delta}{2} \sum_{\substack{ep' \in EP \\ ep' \neq ep}} \sum_{p' \in P} \sum_{p \in P} \left(Fpart_{ep,p,ep',p'} + Fpart_{ep',p',ep,p} \right) + \sum_{r \in R} \sum_{p \in P} \gamma_r Fregpro^{\psi}_{r,ep,p} \right], \tag{24}$$

where besides the same costs as in the model without regeneration, enterprises pay pumping to and from regeneration units, and the cost of regenerating water, depending of the specified outlet concentration. This cost is represented by γ_r. Note that regenerated water cost is non-linear, due to the power $\psi < 1$. In fact, the latter is to take into account that the larger is the volume of water regenerated, the lesser is the operating cost which implies larger regeneration units, and therefore augmented capital costs even if the latter are not taken into account in the present study.

The corresponding MLSFG formulation is defined in Prob. 13, defining the following notation in addition to Eq. (11):

$$\begin{aligned} Fproreg_{ep} &= (Fproreg_{ep,p,r} : 1 \leq p \leq np, \quad 1 \leq r \leq nr) \\ Fregpro_{ep} &= (Fregpro_{r,ep,p} : 1 \leq p \leq np, \quad 1 \leq r \leq nr) \end{aligned} \tag{25}$$

Table 6
Parameters associated with regeneration units.

Regeneration unit type	Parameter	
	C_r^{out}(ppm)	γ_r($/tonne)
1	15	0.85
2	20	0.695
3	30	0.54

$$\min_{\substack{Fpart_{ep}\\Fw\\Fproreg\\Fregpro}} \quad C_{ep}^{tot}(Fpart_{ep}, Fpart_{-ep}, Fw, Fproreg_{ep}, Fregpro_{ep})$$
$$s.t.\begin{cases} Fpart_{ep} \geq 0 \\ (Fw, Fproreg, Fregpro) \quad solve: \\ \min\limits_{\substack{Fw\\Fproreg\\Fregpro}} \quad \sum\limits_{ep \in EP}\sum\limits_{p \in P} Fw_{ep,p} \\ s.t.\ \{\text{Eq. 5, Eq. 17} - \text{Eq. 23} \end{cases} \tag{Prob. 13}$$

As it can be noted, leaders' problems remain unchanged in comparison to the first case, whereas it is not the case for the follower problem. Given the flows between process units which minimize each enterprise's operating cost, the EIP authority determines the minimum freshwater consumption of the EIP by determining the freshwater flowrates to processes, the flowrates from processes to regeneration and flow from regeneration units to processes, as well. Note that this problem is much more complex than the first one, and that any simplifications cannot be done.

The corresponding SLMFG problem is defined as follows (Prob. 14):

$$\min_{\substack{Fw\\Fproreg\\Fregpro\\Fpart}} \quad \sum_{ep \in EP}\sum_{p \in P} Fw_{ep,p}$$
$$s.t.\begin{cases} \text{Eq. 5, Eq .18} - \text{Eq. 21} \\ Fpart_{ep} \quad \text{solves} \quad \forall ep \in EP: \\ \min\limits_{Fpart_{ep}} \quad C_{ep}^{tot}(Fpart_{ep}, Fpart_{-ep}, Fw, Fproreg_{ep}, Fregpro_{ep}) \\ s.t.\ \{\text{Eq. 6, Eq. 17, Eq. 22} - \text{Eq. 23} \end{cases} \tag{Prob. 14}$$

In this case, it is the EIP authority who determines the minimum freshwater consumption in the EIP by choosing *Fw*, *Fregpro* and *Fproreg*. Given the latter, enterprises react by playing a Nash game between them in order to determine their minimum total operating cost.

It is important to make a remark on which agent controls which constraints, in order to successfully model MLFG. Constraints where at least one of the followers' controlled variables appear, have to be part of the follower problem. On the other hand, if in the involved constraint only variables controlled by a given leader are involved, then that constraint is part of that leader problem, e.g. in Prob. 14 the EIP authority's problem consists on constraints where only variables controlled by him are involved, i.e. *Fproreg*, *Fregpro*. Finally, the low-flowrate issue was treated in the same way as in the model without regeneration units.

3.2.1. Case study, results and discussion

All case study parameters of the case without regeneration units still apply to the case with regeneration units (i.e. Tables 2 and 3). In addition, regeneration units operating parameters are illustrated in Table 6. It is assumed that there are 3 different regeneration units which are distinguished by their capacity to regenerate water, i.e. their outlet concentration on contaminant.

Remark that regenerated water cost is superior regarding freshwater cost. Nevertheless, as regenerated water cost is non-linear, it is not always necessarily true that freshwater is cheaper than regenerated water. Regarding the power ψ, it is assumed that when enterprises operate by themselves $\psi = 0.8$ and when they are part of an EIP $\psi = 0.6$. The latter takes into account the fact that by sharing regeneration units in the EIP, and by purifying larger volumes of polluted water capital costs of units would be cheaper. The aforementioned cost-associated parameters were chosen in order to effectively demonstrate the usefulness of the approach adopted in this work.

Results are shown on the same manner regarding the case without water regeneration (Tables 7 and 8).

Optimization problems Prob. 8–Prob. 13 and Prob. 9–Prob. 14 respectively associated to MLSFG and SLMFG have, as again reported by GAMS, 4272 and 612 continuous variables, and 2397 and 270 constraints. Solution times were 6.5 CPUs and 10.9 CPUs.

In Table 8 shared water makes reference to both water sent to other enterprises and also regeneration units. Results of the case study with water regeneration units highlight the importance of the inclusion of regeneration units in the EIP under study. Firstly, it is

Table 7
Results of each enterprise operating by itself with regeneration units.

Enterprise		1	2	3	Total
Water flowrate (tonne/h)	Fresh	98.33	22.00	97.50	217.83
	Regenerated	0.00	38.17	111.46	149.63
Cost (MMUSD/year)	Freshwater + discharge	0.28	0.06	0.27	0.61
	Reused water	0.01	0.02	0.05	0.08
	Regenerated water	0.00	0.08	0.19	0.27
	Total	0.28	0.17	0.51	0.96

Table 8
Summary of results of the EIP with shared regeneration units.

MOO					
Enterprise		1	2	3	Total
Water flowrate (tonne/h)	Fresh	20.00	20.00	122.80	162.80
	Shared	103.82	67.71	84.32	255.85
	Regenerated	89.59	0.00	78.80	168.39
Cost (MMUSD/year)	Freshwater + Discharge	0.02	0.04	0.40	0.46
	Reused water	0.04	0.03	0.05	0.11
	Regenerated water	0.13	0.00	0.09	0.22
	Total	0.19	0.06	0.54	0.79
Nash equilibrium (MLSFG)					
Enterprise		1	2	3	Total
Water flowrate (tonne/h)	Freshwater (tonne/h)	77.10	48.14	94.38	219.62
	Shared	86.38	63.56	124.93	274.87
	Regenerated	23.95	0.00	96.30	120.24
Cost (MMUSD/year)	Freshwater + Discharge	0.17	0.13	0.31	0.61
	Reused water	0.03	0.01	0.04	0.09
	Regenerated water	0.05	0.00	0.11	0.15
	Total	0.24	0.14	0.44	0.83
Nash equilibrium (SLMFG)					
Enterprise		1	2	3	Total
Water flowrate (tonne/hr)	Freshwater (tonne/hr)	20.00	20.00	20.00	60.00
	Shared	126.49	149.54	226.66	502.69
	Regenerated	100.62	64.67	166.64	331.93
Cost (MMUSD/year)	Freshwater + Discharge	0.04	0.02	0.11	0.17
	Reused water	0.04	0.03	0.08	0.15
	Regenerated water	0.12	0.08	0.19	0.39
	Total	0.19	0.13	0.39	0.71

noted that by working standalone (and with given costs) any enterprise can really make benefit of using regeneration units, e.g. enterprise 1 does not use regenerated water at all, whereas freshwater consumed is considerably decreased globally. It is important to note that this kind of results was expected, since cost parameters were chosen on purpose to demonstrate the usefulness of EIPs and MLFG methodology.

On the contrary, when enterprises work in an EIP configuration, the benefit of using water regeneration units is clear. Yet again, MOO results do not provide satisfaction to all players in the EIP given the arbitrary GP parameters, proving the usefulness of the proposed MLFG approach. Regarding the MLSFG results, it is highlighted that all enterprises have noticeable benefits compared to the standalone case, where the solution correspond to an equilibrium state between the operating costs of the three leaders involved, earning respectively 14.53, 13.59 and 14.0%. Total freshwater consumption is decreased regarding the standalone case, as expected, from 314.355 T/h to 219.62 T/h (which means a decrease of 30%). It is important to note that even if e.g. enterprise 2 does not use regenerated water at all, its total operating cost is effectively lowered when other enterprises use regenerated water.

Secondly, the SLMFG results demonstrate that minimum freshwater in the EIP is attained at 60 T/h, by only feeding with freshwater processes which have $Cmax^{in} = 0$. Given the latter, shared and regenerated water are maximized providing all enterprises a relative gain superior to the case of MLSFG, i.e. 31.91, 19.39 and 25.1% respectively. By regenerating the maximum amount of water, its cost is even inferior to that of freshwater, fact which explains the results obtained in the SLMFG case. However, if this amount is not maximized (i.e. results obtained in the MLSFG case) enterprises have lower gains but its solutions are in equilibrium (or at least it corresponds to the solution which satisfies strong stationarity conditions), according to the structure of the game. Again, to be precise, both solutions correspond to different kind of games and do not necessarily correspond to Nash equilibrium but to a solution which satisfies strong stationarity conditions.

An important aspect yet to be addressed is the solution times of the MLFG formulations. For the EIP with regeneration units' case, each optimization problem in the form of Prob. 8 is solved in a matter of seconds to optimality (even if it is solved with BARON to global optimality). By applying the low-flowrate elimination algorithm, the total solution times of the corresponding MLSFG and SLMFG are

5.626 s and 174 s. In fact, the majority of the CPU time is due to achieving the condition where all low-flowrates are eliminated. Moreover, this can be achieved either in the first or in the *n*th outer iteration.

4. Conclusions

In this work, MLFG formulations for the effective design of EIP were successfully addressed. Results underline the effectiveness of the proposed methodology, compared to traditional multi-objective/multi-decision optimization methods, e.g. goal programming. By formulating the problem in a Nash game manner solutions obtained correspond (if solved to optimality) at least to the case where each player objective function value matches the value if the player operates standalone, without having to add additional constraints to the given objective functions. Moreover, the solution obtained corresponds most of the times to an equilibrium solution where all players attain fair gains respectively.

On the other hand, the formulation and proofs provided by Kulkarni and Shanbhag (2014) were numerically proven to be effective and pertinent to MLSFG especially in cases were traditional formulations do not admit equilibrium. In fact, it is also important to note that this kind of formulation (to the best of authors' knowledge) was never modelled and effectively solved in mathematical modelling environments such as GAMS®. In a parallel way, the effectiveness of the solution methods adopted for MLFG was proven to be reliable indeed in medium/large scale problems, solving to optimality this kind of problems in a matter of seconds, even if solution methods do not solve the Nash equilibrium directly but its strong stationarity conditions. Although, it is to be highlighted that the given industrial water network models provided in the present work correspond to a linear model and as a perspective more non-linear models are yet to be solved. However, given the considerable number of complementarity conditions (which are very hard to solve) already included in the MLFG framework, non-linear models of industrial water networks may not pose too much additional efforts. It is furthermore important to notice that SLMFG are easier to solve than MLSFG and generally multi-leader multi-follower games, since there is no need to duplicate follower's conjectures given the nature of a single-leader in the game, which is numerically speaking very convenient. Given the latter, in this work is successfully introduced a reliable alternative to solve chemical/process engineering problems with multiple decision objectives. Moreover, we emphasized that real-world large-scale EIP case studies can be tackled by the methodologies and formulations presented in this work.

It is also important to underline that the introduction of an EIP regulator plays a major role in the above quoted improvements of the EIP integration model since it allows considering MLSFG and SLMFG structures.

Finally, it was also underlined the usefulness of EIPs in the context of industrial symbiosis to produce more sustainable industrial outcomes. The results obtained show that, by unifying efforts, wastes are lowered and effective gain can be achieved. As a perspective, simultaneous energy and water networks will be taken into account with a MLFG approach.

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