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OPTIMAL FINE OF WASTEWATER OUTFALL PROBLEM IN SHALLOW BODY OF WATER: A BILEVEL OPTIMIZATION APPROACH

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Abstract. *This project aims to model the wastewater regulation problem as a bilevel optimization problem. Due to human activities such as industry, agriculture, and domestic use, many bodies of water have been affected by pollution. To remedy the problem of water quality Environmental Protection Agencies use environmental penalty functions. This enforces managers of wastewater treatment plants to find treatment strategies that meet water quality standards before discharging pollution to the environment. In the case of shallow bodies of water, the behavior of the wastewater dispersion is governed by the Navier-Stokes equation; therefore, the objective functions of the decision-makers have a nonlinear behavior relative to a leader-follower dynamic. To find the optimal penalty function we construct the emission concentration system solution and define the wastewater regulation problem as a bilevel optimization problem. The aim of this paper is three-fold: First, it formulates the wastewater regulation problem as a bilevel optimization problem; second, it provides theoretical insight when the problem is reformulated to a single-level formulation using a Karush-Kuhn-Tucker condition approach; third, it develops discretization techniques that allow finding numerical solutions of the location of the wastewater regulation problem.*

Keywords: Multi-agent systems, Operational research in environment and climate change, Nonlinear programming, Pricing

1. **Introduction.** The coastal and maritime districts are constantly unclothed to land-based pollution sources, caused by industrial and domestic activities. Wastewater carries pollutants to the sea by sewage discharging where the concentrations of pollution are decreased by the chemical or biological processes [1]. The management scenario is complex when social and environmental issues are considered and have more than one decision-maker in the system. Adequate decision-making must be based on environmental studies and technical capabilities, including regionally developed solutions with local public participation [2].

This research aims to address the management of the wastewater from the point at which Environmental Protection Agencies (EPA) can impose environmental penalty functions to indirectly enforce regional governments and their treatment plants to select strategies that satisfy water quality standards. In the early days, the environmental insignificant

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penalties had little effect on corporations and individuals to comply with environmental regulations [3]. In 2012 Earnhart and Segerson [4] showed empirically and theoretically that over-enforcement could lead to worse environmental performance.

As shown in Figure 1 at the beginning of the process, the EPA assigns the penalties for violating environmental regulatory standards, then the treatment plants (dischargers) select a managing strategy of the intensity of the purification process and consequently the mass flow of emissions, depending on those emissions and the physical properties of the water body, which is what determines the behavior of the dispersion of pollutants.

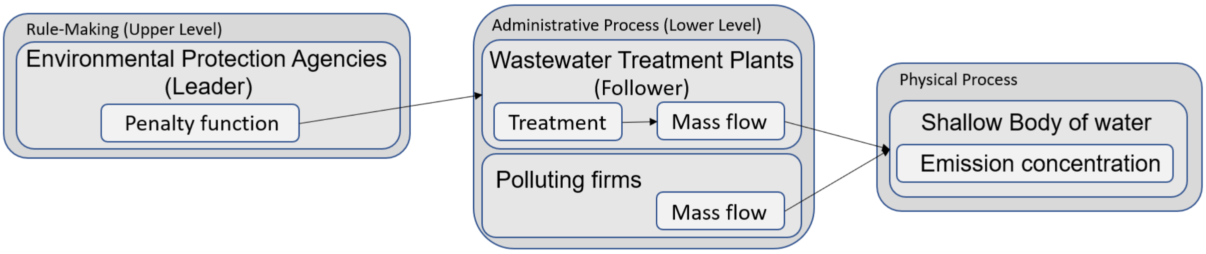

Figure 1. Regulation of wastewater process

The regional government controls directly or indirectly the operative aspects of the wastewaters, but as its objectives are not in conflict with those of the treatment plants they will be taken as a single decision-maker, and then an EPA – Regional Government subsystem is generated. The Regional Government can apply purification treatments to the wastewaters. However, if the environmental regulatory standards problems are not resolved by the end of the period, the EPA penalizes the regional government and their treatment plants. The problem then is to find the penalization function to minimize the environmental impact of the wastewater discharges where the EPA and the Regional Government need to find an equilibrium and it is similar to previous works like [5] that is devoted to the calculation of the equilibrium in the Stackelberg-Nash-Cournot model under special assumptions about the market price function and the agents' cost functions. Some approaches to the problem of assigning a penalty function were handled in other models of wastewater management as [6-8] with the assumptions of lineal environmental damage functions and pollutants discharged into rivers.

This research is based on previous work on the location of wastewater outfall problem [1,9-14] in regard to the dispersion of pollutants and the management of wastewater treatment plants where it has been posed as a multi-objective problem (that tries to optimize two objectives simultaneously) with Pareto solutions [15,16] or Stackelberg strategies as mentioned in [17]. A strong Stackelberg problem corresponds to an optimistic bilevel problem, where a leader player announces his move first taking account of the decisions of the follower player and both try to minimize their cost functions; if the leader chooses any other strategy but the Stackelberg strategy, then the follower will choose a strategy that minimizes its own cost function but the resulting cost for the leader will be greater than or equal to that when the Stackelberg strategy is used by the leader [18].

In previous works, the fine function depends on a damage function as a linear function on the emissions of the treatment plants where the classical expression for the optimal marginal fine should equal the marginal damage divided by the probability of detection, a linear approximation of the damage function might be valid for small emission ranges but is unlikely to hold for larger ranges but it is a good approximation for water bodies like rivers that can be represented as one-dimensional bodies of water. When the damage function is no longer linear it is impossible to assess the impact of one firm only referring to that particular firm's emissions; in the case of interactions with emissions of other firms it will be necessary to take account of the interdependence's between firms, economy, and environment to determine the actual damage occurred and the corresponding penalty function. The mathematical framework of previous works in the location outfall problem is used in this research to find an optimal fine for shallow bodies of water like estuaries, lakes, or coasts that present non-linear functions of damage, a case that has not been treated in previous studies [8].

We aim to address the regulation of the wastewater using a bilevel optimization approach, which is characterized by two levels of hierarchical decision making where the second objective stands as one of the constraints of the first one, as it has been done in other problems with the same hierarchical structure like in previous papers [19-21]. Each independently controls only a set of decision variables and has different conflicting objectives. Each planner attempts to optimize its objective function and is not only affected by the decisions of the other planners but also the lower level planner executes its policies afterward given the decisions of the upper-level planer. These types of practical optimization problems are well explored theoretically, and various practical solution methods exist as shown in [22,23]. However, bilevel optimization problem as the combination of two classical dynamic optimization problems was introduced by [24] and using cost or penalty functions known from solution algorithms for variational inequalities [25] are applied. This new type of optimization problem is not only considerably more difficult to solve but also seeks better modeling of dynamic systems on engineering and economics. Bilevel optimization problems are described in more detail by [24], and some solution methods are explored in [17,26].

The rest of the paper consists of the following sections: the model and the system's behavior are specified in Section 2; in Section 3 the properties of the system and assumptions employed are specified, also Section 3 gives the general model formulation and explains the Karush-Kuhn-Tucker (KKT) conditions reach the single-level reduction; the emission concentration system solution is obtained and the optimal fine reformulation of wastewater outfall problem is given as a single-level Mixed-Integer Nonlinear Problem (MINLP) in Section 4; in Section 5 the final algorithm and its illustrative example are provided; finally, Section 6 draws the conclusions and a possible item of future research.

2. **Formulation and Description of the Optimal Fine of Wastewater Outfall Problem.** Since we do not have direct access to the pollution values, in many cases the environmental models are approximations to fluid dynamical equations which are forced by parameterization of physical processes; this involves multiple sub-models and many parameters. The pollution dispersion model is the Spatio-temporal process which represents the pollution at any location of interest and any time and uses the water flow described by the shallow water equation.

Let us consider a shallow body of water area Ω where every position $s = (x, y) \in \Omega \subset \mathbb{R}^2$ and with edges Γ, within this body of water there are protected areas $A_i \subset \Omega$, where the level of water pollution should not exceed a maximum level of pollution. This can be achieved through proper placement of wastewater treatment plants where the point of submarine sewage discharges is at point $c_i \subset \Omega$. If $\rho(s, t, M)$ denotes the concentration of pollution at point $s \in \Omega$ in the body water area and corresponding mass flow $M = (m_1(t), \ldots, m_{N_e}(t))$ of the polluters, the flow of this sewage in a shallow domain can be modeled by the shallow water equation [27] that is obtained from the incompressible Navier-Stokes equation by assuming pressure is hydrostatic and integrating into depth.

$$\begin{aligned} &\frac{\partial \rho}{\partial t} + \vec{v} \cdot \nabla \rho - \beta \Delta \rho + k\rho = \frac{1}{h} \left(\sum_{i=1}^{N_e} m_i(t) \delta_{c_i}(s) \right), \text{ in } \Theta \\ &\rho(s, 0) = \rho_0(s), \text{ in } \Omega \\ &\frac{\partial \rho}{\partial n} = 0, \text{ in } \Gamma \end{aligned} \tag{1}$$

where the following notation was used to describe the emission concentration system.

Ω: Water body area.
$s = (x, y) \in \Omega$: Coordinate.
T: Tidal cycle.
$t \in [0, T]$: Time.
$\Theta = \Omega \times (0, T)$: Water body area over time.
$\Gamma = d\Omega \times (0, T)$: Edge of the water body over time.
ρ: Depth-averaged emission concentration.
$\vec{v}(s, t) \in [L^\infty(0, T; W^{1,\infty}(\Omega))]^2$: Water horizontal velocity, height-averaged.
$\beta > 0$: Viscosity horizontal coefficient, which considers turbulent effects and dispersion in vertical direction.
k: Experimental value of emissions loss rate.
$h(s, t) \in C\left(\bar{\Omega} \times [0, T]\right)$: Water height, assumed to verify $h(s, t) \geq \alpha > 0$, $\forall (s, t) \in \bar{\Omega} \times [0, T]$.
N_e: Number of pollution emitters.
c_i: Points which discharge wastewater.
$m_i(t)$: Emission mass flow released at point c_i in kg/m^{3}s.
δ_{c_i}: The Dirac value at point $c_i \in \Omega$.
$\rho_0(s) \in C\left(\bar{\Omega}\right)$: Initial emission concentration.
n: Unit outer normal vector to boundary $d\Omega$.

Then the evolution of emission concentration ρ in the water body area over time is described by solving the following boundary problem where $\frac{\partial \rho}{\partial t}$ is the time rate change of total momentum, $\vec{v} \cdot \nabla \rho$ is the net momentum flux, $\beta \Delta \rho$ corresponds to the body forces, $k\rho$ is the loss rate of the emissions and $m_i(t)\delta_{c_i}(s)$ is the $m_i(t)$ mass flow rate of emissions at the point c_i.

In the following subsections, we start defining one of the main level planners (the follower).

2.1. **Management of wastewater outfall problem.** In environmental economics, the emissions of a firm are assumed to express emissions in monetary terms and are assumed to be weakly increasing [28]. This approach is often used in firms where contamination depends on the number of products manufactured, but that approach does not fully meet the needs and conditions of water treatment plants that can share information, cooperate and take account of their interactions.

The public and private corporations should be responsible for dealing with the plant by manipulating the pollution mass flow discharged m to decrease economical costs, both in the purification processes and in the penalties if the Fecal Coliforms (FC) concentration is larger than a certain threshold σ in its influence district A_F.

$$\begin{aligned} \min_{m \in M_{ad}} J_F(m; Z_F) &= \int_0^T J_C(m)dt + \int_0^T J_f(m, Z_F)dt \\ &= \int_0^T \left(J_C(m) + \frac{Z_F}{2} \int_{A_F} [\max(\rho(s, t, M) - \sigma; 0)]^2 ds \right) dt \end{aligned}$$

$$\text{s.t. } m^L \le m(t) \le m^U$$
$$\rho \text{ is the solution of the state system (1)} \tag{2}$$

The following notation was used to describe the management of wastewater outfall problem.

J_{F_i}: Costs of the the plant i.
$M = (m_1(t), \dots, m_{N_e}(t))$ of the polluters.
m: Mass flow emissions of the treatment plant.
m^U: Upper limit of m.
m^L: Lower limits of m.
$M_{ad} = \left\{m \in L^\infty(0,T) : m^U \le m(t) \le m^L \text{ a.e in } (0,T)\right\}$: Set of feasible treatments.
Z_F: Penalty parameter of fine function.
Ω: Water body area.
$s = (x,y) \in \Omega$: Coordinate.
T: Tidal cycle.
$t \in [0,T]$: Time.
J_C: Cost of the purification process.
J_f: Fine cost for insufficient purification.
A_F: Protected area by the treatment plant.
$\rho(s,t,M)$: Depth-averaged emission concentration.
σ: Threshold emission standard.

The treatment cost $J_C \in C^2(0,\infty)$ of the discharge m is a convex function, Z_F is the penalty parameter and decision variable of an EPA and $\max(\rho(s,t,M) - \sigma; 0)$ is the positive part of the difference between emissions and a tolerance threshold σ on which the fine cost J_f is determined. This problem presents technological constraints that limit the intensities of treatment that can be applied on the plants where m^U represents the discharge corresponding to the most intense depuration treatment applied and m^L corresponding to a null depuration.

In the following subsections, we start defining the second main level planner (the leader).

2.2. **Optimal fine of wastewater outfall problem.** The utility functions are used to represent individual preference, by analogy, a single societal utility function represents social choices to serve to construct social preferences. We call such a societal utility function a social welfare function [29]. A social welfare function would give the social utility from a particular bundle. The desirability of two bundles could be compared by comparing the welfare each gives.

In the choice of environmental policy instruments, the firm's compliance decisions depend on the different instruments selected by the government with the intention of maximizing social welfare [8,30] or as in the model used, minimize costs and environmental damage.

Based on the model of Rousseau and Telle [8] consider the damage function as non-linear since it is generated based on the diffusion of pollutants described by the Navier-Stokes equations. In this case, a firm does not produce any good that could be sold in the market, the environmental inspection agency is assumed to check the pollution levels of the plant at all times and the treatment plants are not considered to have an abatement cost since they can choose the pollution that they will emit being a wastewater treatment plant.

$$\min J_L(m, Z_F) = J_F(m, Z_F) + \int_0^T J_D(m)dt + J_I - \int_0^T J_f(m, Z_F)dt$$

$$
\begin{aligned}
&= \int_0^T J_C(m)dt + \int_0^T J_D(m)dt + J_I \\
&= \int_0^T J_C(m)dt + \frac{Z_L}{T|A_L|}\int_0^T \int_{A_L} \rho(s,t,M)dsdt + J_I
\end{aligned}
$$

$$
\begin{aligned}
\text{s.t. } & Z_F^L \le Z_F \le Z_F^U \\
& m \in \Psi(Z_F) \\
& \rho \text{ is the solution of the state system (1)}
\end{aligned}
\tag{3}
$$

The following notation was used to describe the optimal fine of wastewater outfall problem.

$M = (m_1(t), \dots, m_{N_e}(t))$ of the polluters.
J_D: Damage function.
J_I: Inspection cost.
Z_F: Penalty parameter of fine function.
Z_F^U: Upper limit of Z_F.
Z_F^L: Lower limit of Z_F.
Z_L: Penalty parameter of environmental damage.
Ω: Water body area.
$s = (x, y) \in \Omega$: Coordinate.
T: Tidal cycle.
$t \in [0, T]$: Time.
A_L: Protected area of the Environmental Protection Agencies.
$\rho(s, t, M)$: Depth-averaged emission concentration.
$\Psi(Z_F)$: All optimal pairs (m, Z_F) of $J_F(m, Z_F)$ for a fixed Z_F.

A very intuitive summary of the damage is the average behavior of the pollution ρ and used in other environmental problems [31]. We denote this as the aggregated damage variable which corresponds to the normalized total (spatial and temporal) damage (economic, social, and environmental) over region A_L and time T due to a specific M. The normalized temporality-spatially aggregated damage on A_L and time duration T is $J_D(M) = \frac{A_L}{T|A_L|}\int_0^T \int_{A_L} \rho(s,t,M)dsdt$, the quantity $Z_L \int_0^T \int_{A_L} \rho(s,t,M)dsdt$ represents the aggregate damage over a region A_L and time period T and the penalty parameter Z_L represents the importance or the vulnerability to pollution exposure in the region A_L.

The EPA set a penalty function choosing the parameter Z_F seeking to reduce the costs of the treatment plants J_C, reduce the average environmental impact cost J_D in its area of interest A_L over time T and take into account an inspection cost J_I which is a constant value.

2.3. **Bilevel formulation.** In order to obtain the conditions of optimality for the location of wastewater regulation problem (3), we are going to reduce the formulation generally and completely. The idea is to obtain a general formulation for the original problem of interest and applying theoretical results that can provide optimality conditions.

We assume an optimistic situation, in the sense that for every decision of the leader, the follower will choose a strategy among the optimal options which minimizes the scalar objective of the leader, and in this case, the leader will choose a strategy that minimizes the best he can among the best responses of the follower [17].

Let us rewrite problem (3) as an optimistic bilevel optimization problem:

$$\min J_L(m, Z_F) = \int_0^T J_C(m)dt + \frac{Z_L}{T|A_L|}\int_0^T \int_{A_L} \rho(s,t,M)dsdt + J_I$$

s.t. $Z_F^L \leq Z_F \leq Z_F^U$

$m \in \Psi(Z_F)$

where $\Psi(Z_F)$ is the solutions of

$$\min J_F(m; Z_F) = \int_0^T J_C(m)dt + \frac{Z_F}{2}\int_0^T \int_{A_{Fi}} [\max(\rho(s,t,M) - \sigma; 0)]^2 dsdt$$

s.t. $m^L \leq m(t) \leq m^U \quad \forall t \in [0,T]$

$\rho(s,t,M)$ is the solution of the state system (1) (4)

The space is defined as $W := [0,T] \times W_m^{1,1} \times \mathbb{R}$. Then the process $(t, m, Z_F) \in W$ is taken as being feasible for (3) if it fulfills the dynamical system, the initial conditions, and the constraints of a pure state, while (m^*, Z_F^*) shows a solution of global optimal for the problem of the corresponding lower level (management of wastewater outfall problem). Now we define a local minimizer as the following.

Definition 2.1. *Let us use a feasible process $(m^*, Z_F^*) \in W$. Then (m^*, Z_F^*) is a local minimizer of problem* (3) *if there exists $\epsilon > 0$ such that*

$$J_L(m(t)^*, Z_F^*) \leq J_L(m(t), Z_F) \tag{5}$$

holds provided that $(m, Z_F) \in \mathbb{U}^{\epsilon}_{[0,T]\times W_m^{1,1}\times\mathbb{R}}(m^*, Z_F^*)$, and (m, Z_F) is feasible for (3).

In the next section, we study in detail problem (2) and (3) and the assumptions and conditions necessary to find the local minimizer of the problem.

3. **General Settings and Optimality Conditions.** Analyzing the properties of the emission system (1) with regard to the lower-level and upper-level problems, our formulation satisfies that, for each $Z_F \in \left[Z_F^L, Z_F^U\right]$, problem (2) admits a unique solution, and problem (3) admits at least one solution and therefore the existence of a local minimizer of the problem (4).

The existence and regularity solutions of the state system (1) are defined by transposition techniques as described by Alvarez-Vázquez et al. [9] and determine the conditions in which the function (2) is well defined with the following theorem.

Theorem 3.1. *Note that Ω is a bounded domain with a boundary of sufficiently smooth $\partial\Omega$. We consider $h \in C\left(\bar{\Omega} \times [0,T]\right)$ and $\vec{v} \in [L^\infty(0,T; W^{1,\infty}(\Omega))]^2$ which fulfil $h(x,t) \geq \alpha > 0$, $\forall (x,t) \in \bar{\Omega} \times [0,T]$. The following is satisfied,*

1) A unique function $\rho \in [L^r(0,T; (W^{1,s}(\Omega))) \cap L^2(0,T; L^2(\Omega))]$ exists with

$$\frac{\partial \rho}{\partial t} \in L^r\left(0, T; \left(W^{1,s'}(\Omega)\right)'\right),$$

solution of (1) *and verifying.*

$$\int_0^T \left\langle -\frac{\partial \Phi}{\partial t} - \beta\Delta\Phi - div(\Phi\vec{v}) + k\Phi, \rho \right\rangle dt$$

$$= \int_\Omega \Phi(s,0)\rho_0(s)ds + \sum_{i=1}^{N_e}\int_0^T \frac{1}{h(c_i,t)}\Phi(c_i,t)m_i(t)dt,$$

for all $\Phi \in L^2(0,T; H^2(\Omega)) \cap H^1(0,T; L^2(\Omega))$ so that $\beta\frac{\partial\Phi}{\partial n} + \Phi\vec{v}\cdot\vec{n} = 0$ on $\partial\Omega \times (0,T)$, $\Phi(\cdot, T) = 0$ in Ω.

2) If a closed set $E \subset \Omega$ exists such that $\Omega \backslash E$ should be a sufficiently smooth enough domain, $\{c_1, \dots, c_{N_e}\} \subset E$ and $A_L \cup A_F \subset \Omega \backslash E$, then $\rho_{(A_L \cup A_F) \times [0,T]} \in C((A_L \cup A_F) \times [0,T])$, so that the function

$$F : (Z_F, m) \to F(Z_F, m) = \rho_{(A_L \cup A_F) \times [0,T]}$$

is well-defined, continuity and

(a) For each $Z_F \in \left[Z_F^L, Z_F^U\right]$ the function

$$F(Z_F, \cdot) : m \in M_{ad} \to F(Z_F, m) \in C((A_L \cup A_F) \times [0,T])$$

is affine, and Frechet (also Gateaux) differentiable.

(b) If $h \in C([0,T]; C^1(\Omega))$, then, for each $m \in M_{ad}$, the function

$$F(\cdot, m) : Z_F \in \left[Z_F^L, Z_F^U\right] \to F(Z_F, m) \in C((A_L \cup A_F) \times [0,T])$$

is affine, and Gateaux-differentiable.

Assuming that Theorem 3.1 is fulfilled, then we have that $J_F(m, Z_F)$ is well defined in $\left[Z_F^L, Z_F^U\right] \times M_{ad}$, and can be written as

$$J_F(Z_F, m) = J_{FC}(m) + J_{FP}(F(Z_F, m))$$

with $J_{FC} : m \in M_{ad} \to J_{FC}(m) \in \mathbb{R}$, given $J_{FC}(m) = \int_0^T J_C(m) dt$, $J_{FP} : \rho \in C((A_L \cup A_F) \times [0,T]) \to J_{FP}(\rho) \in \mathbb{R}$, defined by

$$J_{FP}(\rho) = \int_0^T J_P(m, Z_F) dt = \frac{Z_F}{2} \int_0^T \left(\int_{A_F} [\max(\rho(s,t,M) - \sigma; 0)]^2 ds \right) dt.$$

As shown in Theorem 2 in [9], supposing the hypotheses given in Theorem 3.1, if $J_C \in C(0,\infty)$ is convex strictly, then, for each $Z_F \in \left[Z_F^L, Z_F^U\right]$, problem (2) has uniquely a solution m_b, with this the problem (3) is well-posed by and let us use the function

$$\Xi : Z_F \in \left[Z_F^L, Z_F^U\right] \to \Xi(Z_F) = m_{Z_F} \in M_{ad}, \tag{6}$$

where m_{Z_F} is the solution of problem (2). The following lemma ensures the continuity of Ξ.

Lemma 3.1. *Let $Z_F \in \left[Z_F^L, Z_F^U\right]$ and let $\{m^n\} \subset M_{ad}$ be a sequence with $\{m^n\} \to m$ (convergence in the weak* topology of $L^\infty(0,t)$). By means of the hypotheses of Theorem 3.1 we result in that $\{F(Z_F, m^n)\} \to F(Z_F, m)$ in $C((A_L \cup A_F) \times [0,T])$.*

This leads to the following result demonstrated in [9].

Theorem 3.2. *Let us assume that $f \in C(0,\infty)$ is convex strictly and that Theorem 3.1 hypotheses are fulfilled. Then the function Ξ, obtained by (6), is continuous in M_{ad}, considering the weak* topology of $L^\infty(0,T)$.*

If the following composition of functions is taken into account:

$$\left[Z_F^L, Z_F^U\right] \to \left[Z_F^L, Z_F^U\right] \times M_{ad} \to \mathbb{R},$$
$$Z_F \to (Z_F, m_{Z_F}) \to J_L(Z_F, m_{Z_F})$$

and define

$$J = J_L \circ \left(1_{\left[Z_F^L, Z_F^U\right]} \times \Xi\right),$$

then problem (3) can be rewritten as

$$\min_{Z_F \in [Z_F^L, Z_F^U]} J(Z_F) = \int_0^T J_C(m) dt + J_{LP}(F(Z_F, \Xi(Z_F))) + J_I \tag{7}$$

where

$$J_{LP} : \rho \in C((A_L \cup A_F) \times [0,T]) \to J_{LP}(\rho) = \frac{Z_L}{T|A_L|} \int_0^T \int_{A_L} \rho(s,t) ds dt \in \mathbb{R}$$

Theorem 3.3. *Suppose that $J_C \in C(0,\infty)$ is convex strictly, and that Theorem 3.1 hypotheses are fulfilled. Then, J is a continuous functional.*

If $J_C \in C(0,\infty)$ is convex strictly, and $\left[Z_F^L, Z_F^U\right] \in \mathbb{R}$ is closed, then the hypotheses of Theorem 3.1 make the problem (7) (or equivalently admit problem (3)), one solution at least.

When functions f and h are assumed to have additional regularity, it enables us to obtain a first-order optimality condition for problem (7). Let us introduce the following problem which is called the adjoint state in the leader problem:

$$\begin{aligned} & -\frac{\partial p}{\partial t} - \beta \Delta p - div(p\vec{v}) + kp = \frac{1}{T|A_L|}\chi_{A_L}, \text{ in } \Theta \\ & p(s,T) = 0, \text{ in } \Omega \\ & \beta \frac{\partial p}{\partial n} + p(\vec{v} \cdot \vec{n}) = 0, \text{ on } \Gamma \end{aligned} \tag{8}$$

This problem accepts a unique solution $L^\infty(\Omega) \cap L^\infty[0,T]$; $\rho \in W^{1,\infty}([0,T]; W^{2,\infty}(\Omega))$ as shown in [32]. Then, Green's formula and integration make (8) give the following result by means of taking account of Lemma 3.1 and Theorem 3.2:

$$\begin{aligned} J_{FP}(\rho) &= \frac{Z_L}{T|A_L|} \int_0^T \int_{A_L} \rho(s,t) ds dt \\ &= Z_L \int_0^T \int_\Omega \frac{1}{T|A_L|} \chi_{A_L} \rho(s,t) ds dt \\ &= Z_L \int_0^T \int_\Omega \left(-\frac{\partial p}{\partial t} - \beta \Delta p - div(p\vec{v}) + kp \right) \rho(s,t) ds dt \\ &= Z_L \left[\int_0^T \int_\Omega \left(\frac{\partial \rho}{\partial t} + \vec{v} \cdot \nabla \rho - \beta \Delta \rho + k\rho \right) p(s,t) ds dt \right. \\ &\quad + \int_0^T \int_{\partial\Omega} \left(\rho p \vec{v} \cdot \vec{n} + \beta p \frac{\partial \rho}{\partial n} - \beta \rho \frac{\partial p}{\partial n} \right) d\gamma dt - \int_\Omega \rho(s,T) p(s,T) ds \\ &\quad \left. + \int_\Omega \rho(s,0) p(s,0) ds \right] \end{aligned}$$

This manipulation changes (7) into

$$J(Z_F) = \int_0^T J_C(m) dt + J_{LP}(F(Z_F, \Xi(Z_F))) + J_I \tag{9}$$

In order to obtain the condition of optimality, the basic property of real functions is required as follows.

Lemma 3.2. *If $f \in C^2(0,\infty)$ is convex strictly, and $D \subset \mathbb{R}$ shows the f' image, that is $D = \{y \in \mathbb{R} : \exists x \in (0,\infty)/y = f'(x)\}$, then f' is invertible, and the inverse function $g = f(f')^{-1} \in C^1$ verifies: $g'(f'(x)) = 1/f''(x)$, $\forall x \in (0,\infty)$.*

Then the following result denotes the condition that should be verified by any problem of bilevel optimization.

Theorem 3.4. *Let us assume that all the hypotheses in Theorem 3.1 are verified and that* $\left[Z_F^L, Z_F^U\right]$ *is a convex set,* $h \in C\left([0,T]; C^1\left(\bar{\Omega}\right)\right)$ *and* $f \in C^2(0,\infty)$ *is strictly convex. Then, if* $(Z_F, m_{Z_F}) \in \left[Z_F^L, Z_F^U\right] \times M_{ad}$ *is a solution for our problem, there exist* $\rho \in [L^r(0,T; W^{1,s}(\Omega)) \cap L^2(0,T; L^2(\Omega))]$ $(r, s \in [1,2),\ \frac{2}{r} + \frac{2}{s} > 3)$ *and* $q \in W^{1,\infty}([0,T]; L^\infty(\Omega)) \cap L^\infty([0,T]; W^{2,\infty}(\infty))$ *satisfying (1), and*

$$f'(m_{Z_F}(t)) + \frac{1}{h(Z_F,t)} q(Z_F,t) = 0, \quad \forall t \in (0,T). \tag{10}$$

In addition, if $p \in W^{1,\infty}([0,T]; L^\infty(\Omega)) \cap L^\infty([0,T]; W^{2,\infty}(\Omega))$ *is the solution of (8) then, for all* $Z_F^* = \in \left[Z_F^L, Z_F^U\right]$*, it verifies*

$$\left(Z_F - a + Z_L \int_0^T \left(\frac{h\frac{\partial p}{\partial Z_F} - p\frac{\partial h}{\partial Z_F}}{h^2}(Z_F,t) m_{Z_F}(t) - \frac{p\left(h\frac{\partial q}{\partial Z_F} - q\frac{\partial h}{\partial Z_F}\right)}{h^3}(Z_F,t)\frac{1}{f''(m_{Z_F}(t))}\right) dt\right)(Z_F - Z_F^*) \geq 0. \tag{11}$$

3.1. **Bilevel optimization problem.** To present a general problem formulation of the upper level has a problem of optimization with Lagrange-type cost function, we rewrite it as an optimistic bilevel optimization problem.

$$\begin{aligned} & J_L := \int_0^T F(t, m(t), Z_F) dt \to \max_{m, Z_F} \\ & G(Z_F) \leq 0 \\ & m(t) \in \Psi(Z_F) \text{ for all } t \in [0,T] \end{aligned} \tag{12}$$

where Ψ represents the solution-set-mapping of the following optimization problem with pure state constraints.

$$\begin{aligned} & J_F := \int_0^T f(t, m(t), Z_F) dt \to \min_{m} \\ & g(t, m(t)) \leq 0 \end{aligned} \tag{13}$$

The following assumptions must be fulfilled within the model (4) [33]:

(A1) $Z_F \in \left[Z_F^L, Z_F^U\right] \subset \mathbb{R}$ and $m(t) \in M_{ad}$ $\forall t$, $\left[Z_F^L, Z_F^U\right]$ and M_{ad} are closed;

(A2) $U : [0,T] \to \mathbb{R}^{m_u}$ is a nonempty compact valued set-valued map. The graph (U) denoted by GrU, is $L \times B$ measurable, where $L \times B$ denotes the σ-algebra of subsets of $[0,T] \times \mathbb{R}^{m_u}$ generated by product sets $M \times N$ where M is a Lebesgue measurable subset of $[0,T]$ and N is a Borel subset of $\mathbb{R}^{m_u}$;

(A3) There exists an $M \times N$-measurable real-valued function k defined on GrU such that for each $t \in GrU$, the functions $\phi(t,\cdot,\cdot)$, $F(t,\cdot,\cdot)$, $G(t,\cdot,\cdot)$ are locally Lipschitz of rank $k(t)$, where $k(t)$ is an integrable function. For each $(m, Z_F) \in \mathbb{R}^{m_x} \times \mathbb{R}$, the functions $\phi(\cdot, m, Z_F) : [0,T] \times \mathbb{R}^{m_u} \to \mathbb{R}^{m_x}$, $F(\cdot, m, Z_F) : [0,T] \times \mathbb{R}^{m_u} \to \mathbb{R}$, $G(\cdot, m, Z_F) : [0,T] \times \mathbb{R}^{m_u} \to \mathbb{R}$ are $L \times B$ measurable;

(A4) The functions $f, g : \mathbb{R}^{m_x} \to \mathbb{R}$ are Lipschitz continuous locally;

(A5) For any $Z_F \in \left[Z_F^L, Z_F^U\right]$, $J_F(Z_F)$ has an admissible pair $(Z_F, m(t))$.

3.2. **Karush-Kuhn-Tucker conditions approach.** The KKT-conditions of nonlinear optimization problems are an approach that in a bilevel problem substitute the lower level problem by its KKT-conditions to obtain a one-level problem with equilibrium constraints.

Definition 3.1. *For the objetive function of upper-level (leader) $F : \mathbb{R}^n \times \mathbb{R}^m \to \mathbb{R}$ and the lower-level (follower) objetive function $f : \mathbb{R}^n \times \mathbb{R}^m \to \mathbb{R}$, the bilevel problem is defined by*

$$\begin{aligned} &\min_{x_l \in X_L, x_f \in X_F} F(x_l, x_f) \\ &\text{s.t. } G_k(x_l, x_f) \leq 0, \quad k = 1, \ldots, K \\ &\qquad x_f \in \Psi(x_l) = \arg\min_{x_f \in X_F} \{f(x_l, x_f) : g_j(x_l, x_f) \leq 0, j = 1, \ldots, J\} \end{aligned} \tag{14}$$

where G_k are the constraints of the upper level, g_j denote the lower level constraints and $\Psi(x_l)$ describes the constraint given by the optimization problem of lower-level and can be understood as a range-constraint parameterization of the decision vector x_f of lower-level.

Optimistically, if multiple optimal solutions of lower level exist, the leader requires the follower to select that solution from the optimal set $\Psi(Z_F)$, which results in the best value of the objective function at the upper level. Some extent of cooperation is assumed between the two players and the optimistic formulation is assured to obtain an optimal solution through a reasonable assumption of regularity and compactness [34].

Theorem 3.5. *If F, f, G_k and g_j are smooth sufficiently, the constraint district Φ in the optimization problem of bilevel is non-empty and compact, and the Mangasarian-Fromowitz Constraint Qualification (MFCQ) is satisfied at all points, then the problem is guaranteed to obtain an optimistic bilevel optimum under the condition that a feasible solution exists.*

The necessary and sufficient conditions for optimality are satisfied when the following hold: f and g are continuously differentiable and convex with respect to x_f with fixed x_l and the MFCQ condition is satisfied.

Definition 3.2. *Given a nonlinear optimization problem (NLP) in the form $\min_{x \in X} f(x)$ s.t. $X = \{x \in \mathbb{R}^n | g_j(x) \leq 0, h_i(x) = 0\}$, with f, g_j, h_i: $\mathbb{R}^n \to \mathbb{R}$ continuously diferentiable functions, where the feasible set of NLP will be denoted by Ω. For a feasible point $\bar{x} \in \Omega$, the Mangasarian-Fromovitz Constraint Qualification (MFCQ) holds at $\bar{x}$ if $\nabla h_j(\bar{x})$ are linearly independent and there exists a vector $d \in \mathbb{R}^n$ such that $\nabla h_j(\bar{x})^T d = 0$ $\forall j$ and $\nabla g_i(\bar{x})^T d < 0$ ($i \in I(\bar{x})$, $I(\bar{x}) := \{i | g_i(\bar{x}) = 0\}$).*

To ensure the optimality of problem bilevel optimization problem (12) we need that the lower-level problem (2) to satisfy the MFCQ conditions, the functions $J_F(m, Z_F)$, subject to inequality constraints $m(t) - m^U \leq 0$ and $m^L - m(t) \leq 0$, are continuously differentiable and convex with respect to $m^{\Delta t}$ fixed Z_F under the hypotheses in Theorem 3.1 and without equality constraints it is trivial that MFCQ conditions are satisfied.

3.3. **Single-level reduction.** When the problem of the lower level is convex and regular sufficiently, it enables us to replace the optimization problem of the lower level under its Karush-Kuhn-Tucker (KKT) conditions. The KKT conditions play a pivotal role in solving a Lagrangian and complementarity constraints and shrink the optimization of the overall bilevel problem to a constrained optimization problem of single-level [35]. For instance, the problem in Definition 3.1 can be changed to the following, when the convexity and regularity conditions are satisfied at the lower level:

$$\begin{aligned} &\min_{x_l \in X_L, x_f \in X_F, \lambda} F(x_l, x_f) \\ &\text{s.t. } G_k(x_l, x_f) \leq 0, \quad k = 1, \ldots, K, \\ &\qquad \nabla_{x_f} L(x_l, x_f, \lambda) = 0, \end{aligned}$$

$$
\begin{aligned}
&g_j(x_l, x_f) \leq 0, \quad j = 1, \dots, J, \\
&\lambda_j g_j(x_l, x_f) \leq 0, \quad j = 1, \dots, J, \\
&\lambda_j \geq 0, \quad j = 1, \dots, J
\end{aligned} \tag{15}
$$

where

$$
L(x_l, x_f, \lambda) = f(x_l, x_f) + \sum_{j=1}^{J} \lambda_j g_j(x_l, x_f).
$$

Still, an optimization task of a single level problem, the formulation given above is not simple necessarily to manipulate. The Lagrangian constraints can be taken as non-convexities even though the conditions of suitable convexity are dealt with on all the objectives and constraints in the formulation of bilevel. The condition of complementarity, inherently being combinatorial, renders the optimization problem of single-level as the following mixed integer program.

4. **Model Discretization and Its Application.** To apply the KKT method is necessary to discretize the functions $M = (m_1(t), \dots, m_{N_e}(t))$ as a variable of finite dimension $M^{\Delta t} = (m_{1,1}, m_{1,2}, \dots, m_{1,N_t}, \dots, m_{N_e,1}, m_{N_e,2}, \dots, m_{N_e,N_t})$. On the other hand, the emission status system of emissions modeled from the Navier-Stokes equations has no analytical solution, so it is necessary to carry out a process of discretization of the variables of time and the area of the water body Ω.

4.1. **Discretization of emission concentration system.** The method of characteristics considers the following equality:

$$
\frac{D\rho}{Dt}(s,t) = \frac{\partial \rho}{\partial t} + \vec{v}\,\nabla\rho = \frac{\partial \rho}{\partial t}(S(s,t;\tau),\tau)_{\tau=t}
$$

$\tau \to S(s,t;\tau)$ is the characteristic line, providing the position at time τ of the particle that occupied the position s at time t.

4.1.1. *Time discretization.* For the time interval $[0,T]$ we choose $N_t \in \mathbb{N}$, $\Delta t = T/N_t$, we define $t_n = n\Delta t$, $n = 0, 1, \dots, N_t$. If we denote $S^n(s) = S(s, t_{n+1}; t_n)$, then the total derivative of ρ at instant t_{n+1} can be approximated by

$$
\frac{D\rho}{Dt}(s, t_{n+1}) \simeq \frac{\rho^{n+1}(s) - \rho^n(S^n(s))}{\Delta t}
$$

The semi-discretized problem is that for each $n = 0, 1, 2, \dots, N-1$, we must find the function $\rho^{n+1}(s)$ satisfying

$$
\begin{aligned}
&\frac{\rho^{n+1} - \rho^n \circ S^n}{\Delta t} - \beta\Delta\rho^{n+1} + \kappa\rho^{n+1} = \frac{1}{h}\left(\sum_{i=1}^{N_e} m_i(t_n)\delta_{c_i}(s)\right) \\
&\frac{\partial \rho^{n+1}}{\partial n} = 0 \\
&\rho(s,0) = \rho_0(s)
\end{aligned} \tag{16}
$$

4.1.2. *Space discretization.* Let us discuss the semi-discretized problem as a variational formulation and we approximate it by using a Lagrange $\mathbb{P}_1$ finite element. Assume Ω means of a polygonal approximation Ω_h. Let $\tau_h(s_j)$ be a triangular approximation of domain Ω_h with vertices $\{s_j : j = 1, \dots, N_v\}$. To each element N_k of a triangle $K \in \tau_h$ we associate two parameters: $v(K)$ denoting the diameter of the set K and $\sigma(K)$ which represents the diameter of the incircle of set K. A triangular approximation τ_h is acceptable if $h \geq \max_{K \in \tau_h} v(K)$ and two positive constants v_t and σ_t are satisfied such that $\frac{v(K)}{\sigma(K)} \leq \sigma_t$ and $\frac{h}{v(K)} \leq v_t$, $\forall K \in \tau_h$.

If the polynomial function piece-wisely in $W^{1,s}(\Omega_h)$ is continuous, we estimate $W^{1,s}(\Omega_h)$ approximately by

$$V_h = \left\{\nu_h \in C^0\left(\bar{\Omega}\right) : \nu_{h|K} \in \mathbb{P}_1 \; \forall K \in \tau_h\right\}$$

and from the formulation of direct variation (16), we reached the following fully discrete approximation of the state system. Given $\rho_{h0} \in V_h$, $\rho_{h0} \approx \rho_0(s)$, find $\rho_h^n \in V_h$ ($\rho_h^n \simeq \rho^n$) for $n = 0, \ldots, N_t - 1$, such that, for all $\nu_h \in V_h$, the following system is valid:

$$\int_{\Omega_h} \frac{\rho_h^{n+1} - \rho_h^n \circ S_h^n}{\Delta t} \nu_h ds + \beta \int_{\Omega_h} \nabla \rho_h^{n+1} \cdot \nabla \nu_h ds + \kappa \int_{\Omega_h} \rho_h^{n+1} \nu_h ds$$
$$= \frac{1}{h} \int_{\Omega_h} \left(\sum_{i=1}^{N_e} m_i(t_n) \delta_{c_i}(s) \nu_h \right) ds \tag{17}$$

where S_h^n is the approximation of S^n, i.e., $S_h^n(s) = s - \Delta t \vec{v}^n(s)$, with $\vec{v}^n = \vec{v}(., t^n)$.

4.1.3. *Convergence analysis.* In studying the numerical convergence of our full discretization problem (17), it is a main difficult point to handle the Dirac measure in the right-hand of the system. Therefore, the usual estimates cannot be employable. To remove this trouble, we apply an approximation to the problem [10].

That is, we approximate each measure $\delta_{c_i}(s)$ by a smooth function $\delta_{hc_i} \in L^2(\Omega)$ satisfying the following properties [10,11]:

1) δ_{hc_i} is null outside the triangle K_i in which c_i lies;
2) $\int_{\Omega_h} \delta_{hc_i}(s) \nu_h(s) ds = \nu_h(c_i)$, $\forall \nu_h \in V_h$;
3) $||\delta_{hc_i} - \delta_{c_i}(s)||_{M(\Omega)} = O(h)$.

Substituting $\delta_{c_i}(s)$ by δ_{hc_i}

$$\int_{\Omega_h} \frac{\rho_h^{n+1} - \rho_h^n \circ S_h^n}{\Delta t} \nu_h ds + \beta \int_{\Omega_h} \nabla \rho_h^{n+1} \cdot \nabla \nu_h ds + \kappa \int_{\Omega_h} \rho_h^{n+1} \nu_h ds$$
$$= \frac{1}{h} \left(\sum_{i=1}^{N_e} m_i(t_n) \nu_h(c_i) \right) \tag{18}$$

4.1.4. *Solution of the emission concentration system.* The resultant discretized problem for each time step is equivalent to a linear system where each equation in the system depends on exactly one variable $\rho_h^{n+1}(S_i)$ as follows [12,13,36]:

$$M_h \rho_h^{n+1} = q_h^n, \; n = 0, \ldots, N_t - 1. \text{ For a given } \rho_h^0,$$
$$\rho_h^{n+1} = \left(\rho_h^{n+1}(s_1), \ldots, \rho_h^{n+1}(s_{N_v})\right)^\top,$$
$$(M_h)_{ij} = \beta \int_{\Omega_h} \nabla \tilde{\nu}_i \nabla \tilde{\nu}_j ds + \left(\frac{1}{\Delta t} + \kappa\right) \int_{\Omega_h} \tilde{\nu}_i \tilde{\nu}_j ds,$$
$$(q_h^n)_l = \frac{1}{\Delta t} \int_{\Omega_h} \left(\rho_h^n \circ S_h^n\right) \tilde{\nu}_l ds + \frac{1}{h} \int_{\Omega_h} \left(\sum_{j=1}^{N_e} m_j(t_n) \delta_{c_j}(s) \tilde{\nu}_l \right) ds,$$

where $\{\tilde{v}_1, \ldots, \tilde{v}_{N_v}\}$ is a basis of V_h, satisfying the following,

$$\tilde{\nu}_i(s_j) = \delta_{i,j} = \begin{cases} 1, & \text{if } i = j \\ 0, & \text{if } i \neq j \end{cases}.$$

The basis functions that provide the shape functions are defined as follows: Be the point $s = (x, y)$, $S_i = (x_i, y_i)$, for each $\{K_r : r = 1, \dots, N_k\}$ triangle with vertices S_A, S_B and S_C, where $0 \le \tilde{\nu}_i(r, s) \le 1$ and $\tilde{\nu}_A(r, s) + \tilde{\nu}_B(r, s) + \tilde{\nu}_C(r, s) = 1$.

$$\tilde{\nu}_i(r,s) = \begin{cases} 1 - \xi - \zeta = \dfrac{1}{2A_{ABC}}(\alpha_A + \beta_A x + \gamma_A y), & \text{if } i = A \\ \xi = \dfrac{1}{2A_{ABC}}(\alpha_B + \beta_B x + \gamma_B y), & \text{if } i = B \\ \zeta = \dfrac{1}{2A_{ABC}}(\alpha_C + \beta_C x + \gamma_C y), & \text{if } i = C \\ 0, & \text{if } i \neq \{A, B, C\} \end{cases}$$

$$A_{ABC} = \frac{1}{2}(x_B y_C + x_C y_A + x_A y_B - x_B y_A - x_C y_B - x_A y_C),$$
$$\alpha_A = x_B y_C - x_C y_B, \quad \beta_A = y_B - y_C, \quad \gamma_A = x_C - x_B,$$
$$\alpha_B = x_C y_A - x_A y_C, \quad \beta_B = y_C - y_A, \quad \gamma_B = x_A - x_C,$$
$$\alpha_C = x_A y_B - x_B y_A, \quad \beta_C = y_A - y_B, \quad \gamma_C = x_B - x_A.$$

The first derivatives of the basis functions are

$$\nabla\tilde{\nu}_i(r,s) = \begin{cases} \left[\dfrac{\beta_i}{2A_{ABC}}, \dfrac{\gamma_i}{2A_{ABC}}\right], & \text{if } i = \{A, B, C\} \\ [0, 0], & \text{if } i \neq \{A, B, C\} \end{cases}$$

To perform the integrals over the polygon Ω_h, it is calculated as the sum of the integrals over each triangle K_r. To calculate the integral over arbitrary triangles, we proceed to make a change of coordinates $[x', y']$ where $S'_A = (0, 0)$, $S'_B = (1, 0)$, $S'_C = (0, 1)$.

$$\begin{aligned} \int_{\Omega_h} f(s)ds &= \sum_{r=1}^{N_k} \int_{K_r} f_r(x, y)dydx \\ &= \sum_{r=1}^{N_k} |J_{rg}(x', y')| \int_0^1 \int_0^{1-x'} f_r(x_r(x', y'), y_r(x', y'))dy'dx' \end{aligned}$$

The linear system of the discrete problem is equivalent to

$$M_h \rho_h^{n+1} = q_h^n,\ n = 0, \dots, N_t - 1. \text{ For a given } \rho_h^0 \tag{19}$$
$$\rho_h^{n+1} = \left(\rho_h^{n+1}(s_1), \dots, \rho_h^{n+1}(s_{N_v})\right)^\top \tag{20}$$
$$(M_h)_{ij} = \beta \sum_{r=1}^{N_k} \int_{K_r} \nabla\tilde{\nu}_i(r,s) \cdot \nabla\tilde{\nu}_j(r,s)ds + \left(\frac{1}{\Delta t} + \kappa\right) \sum_{r=1}^{N_k} \int_{K_r} \tilde{\nu}_i(r,s)\tilde{\nu}_j(r,s)ds \tag{21}$$
$$(q_h^n)_l = \frac{1}{\Delta t} \sum_{r=1}^{N_k} \int_{K_r} \rho_h^n(s - \Delta t \vec{v}^n(s))\tilde{\nu}_l(r,s)ds + \frac{1}{h}\left(\sum_{j=1}^{N_e} m_j(t_n)\nu_l(r_{c_j}, c_j)\right) \tag{22}$$

The solution of this linear system can be obtained by usual methods like matrix solution:

$$\rho_h^{n+1} = (M_h)^{-1} q_h^n, \quad n = 0, 1, \dots, N_t - 1. \tag{23}$$

From this, for each vertex $\{s_j : j = 1, \dots, N_v\}$ of the triangulation of domain Ω_h, we can describe the emission concentration ρ_{hj}^n that depends on the variables $m^{\Delta t}$.

For each triangle $\{K_r : r = 1, \dots, N_k\}$, be $s = (x, y)$ an interior point of the triangle K_r with vertices S_A, S_B and S_C, we can describe the emission concentration in s as follows.

$$\rho_{hr}^n\left(s, M^{\Delta t}\right) = \rho_{hA}^n\left(M^{\Delta t}\right)\tilde{\nu}_A(r,s) + \rho_{hB}^n\left(M^{\Delta t}\right)\tilde{\nu}_B(r,s) + \rho_{hC}^n\left(M^{\Delta t}\right)\tilde{\nu}_C(r,s)$$

We consider $\rho_0 = 0$, $\forall s \in \Omega$.

4.2. **Discretized single-level reduction.** To apply the KKT conditions (15) it is necessary to obtain discrete problems equivalent to (2) and (3), we consider the previous time discretization and define

$$L^{\Delta t} = \left\{ f^{\Delta t} \in L^\infty(0,T) : f^{\Delta t}|_{(t^{n-1},t^n]} \in P^0, \text{ for } n = 1, \ldots, N \right\}.$$

The set M is approximated by the finite dimension space $M^{\Delta t} = M \cap L^{\Delta t}$, with this we can define the following equivalent function:

$$\begin{aligned} J_F(m, Z_F) &\simeq J_{Fh}\left(m^{\Delta t}, Z_F\right) \\ &= \Delta t \sum_{n=1}^{N_t} \left(J_C\left(m^{\Delta t}\right) + \frac{Z_F}{2} \sum_{r=1}^{N_{A_F}} \int_{K_{A_{Fr}}} \left[\max\left(\rho^n_{hA_{Fr}}\left(s, M^{\Delta t}\right) - \sigma; 0\right)\right]^2 ds \right) \end{aligned}$$

For the evaluation of J_L, for each $Z_F \in \left[Z_F^L, Z_F^U\right]$, we can approximate

$$\begin{aligned} J_L(m, Z_F) &\simeq J_{Lh}\left(m^{\Delta t}, Z_F\right) \\ &= \Delta t \sum_{n=1}^{N_t} \left(J_C\left(m^{\Delta t}\right) + \frac{Z_L}{T|A_L|} \sum_{r=1}^{N_{A_L}} \int_{K_{A_{Lr}}} \rho^n_{hA_{Lr}}\left(s, M^{\Delta t}\right) ds \right) + J_I \end{aligned}$$

where, for $n = 1, \ldots, N$, ρ_h^n is obtained by the solution (23) of the linear system (19). Once the KKT conditions are applied, the single-level problem obtained as an MINLP problem is obtained.

$$\begin{aligned} \min J_{Lh}\left(m^{\Delta t}, Z_F\right) = {} & \Delta t \sum_{n=1}^{N_t} J_C\left(m^{\Delta t}\right) + \frac{Z_L}{T|A_L|} \Delta t \sum_{n=1}^{N_t} \left(\sum_{r=1}^{N_{A_L}} \int_{K_{A_{Lr}}} \rho^n_{hA_{Lr}}\left(s, M^{\Delta t}\right) ds \right) \\ & + J_I \\ \text{s.t. } & Z_F - Z_F^U \le 0 \\ & Z_F^L - Z_F \le 0 \\ & \nabla_{m^{\Delta t}} \left(J_{Fh}\left(m^{\Delta t}, Z_F\right) + \sum_{n=1}^{N_t} \left(\lambda_{t_n} \left(m^{\Delta t}(t_n) - m^U\right) - \lambda_{N_t + t_n} \left(m^{\Delta t}(t_n) - m^L\right)\right) \right) = 0 \\ & m^{\Delta t}(t_n) - m^U \le 0 \\ & m^L - m^{\Delta t}(t_n) \le 0 \\ & \lambda_{t_n}(m^{\Delta t}(t_n) - m^U) \le 0 \\ & \lambda_{N_t+t_n}\left(m^L - m^{\Delta t}(t_n)\right) \le 0 \\ & \lambda_{t_n} \ge 0 \\ & \lambda_{N_t+t_n} \ge 0 \end{aligned} \tag{24}$$

where the discrete function J_{Fh} is equal to

$$\begin{aligned} J_{Fh}\left(m^{\Delta t}, Z_F\right) = {} & \Delta t \sum_{n=1}^{N_t} J_C\left(m^{\Delta t}(t_n)\right) \\ & + \Delta t \frac{Z_F}{2} \sum_{n=1}^{N_t} \sum_{r=1}^{N_{A_F}} \int_{K_{A_{Fr}}} \left[\max\left(\rho^n_{hA_{Fr}}\left(s, M^{\Delta t}\right) - \sigma; 0\right)\right]^2 ds \end{aligned} \tag{25}$$

If the constraints set is nonempty, then the discretized problem (24) has, at least, one solution since the interval $\left[Z_F^L, Z_F^U\right]$ is compact and the cost function is trivially continuous. The next step is the use of numerical methods for the resolution of the discretized problem.

5. Numerical Implementation and Results.

The computation of the discrete single-level reduction problem (24) is an MINLP problem that is solved using the solvers IPOPT (Interior Point Optimizer) and APOPT (Advanced Process OPTimizer). We need to know previously the emission concentration ρ_h, solution of (17), we use symbolic algebra in Matlab ©R2020a to solve systems of linear equations dependent on $M^{\Delta t}$ (23), once with functions that represent the solutions of ρ_h for all vertices and time steps, we proceed to build the model file that represents the problem (24) which was sent to solve using APMonitor.

APMonitor Optimization Suite is a freely available software for solutions of linear programming, quadratic programming, nonlinear programming, and mixed-integer (MILP and MINLP) problems [37]; MINLP problems can be solved by large-scale optimizers such as the active-set Sequential Quadratic Programming solver APOPT that uses Branch and Bound method to find solutions in the case of restricted variables to integers values [38]. The solver has an excellent scaling with an increased number of controlled variables but poor computational scaling with an increased number of decision variables and adds the advantage to quickly find a solution from a nearby candidate solution [39].

5.1. Algorithm.

1) Loading the corresponding triangulation and parameters as appropriate matrices and vectors.
2) Calculate the matrix M_h (21).
3) For each $n = 1, 2, \dots, N_t$:
   - With symbolic algebra construct a vector of equations q_h^n (22) dependant of m.
   - Construct the matrix ρ_h^{n+1} dependant of m solving the linear system (23).
4) Construct the function J_{Fh} (25) using the functions ρ_h.
5) Construct the function J_{Lh} using the functions ρ_h.
6) Construct the model (24) for APMonitor.
   - Model parameters used:
     minlp_maximum_iterations = 10000
     minlp_max_iter_with_int_sol = 1000
     minlp_branch_method = 3
     minlp_gap_tol = 1.0×10^{-2}
     minlp_integer_tol = 1.0×10^{-2}
     minlp_integer_max = 2.0×10^{9}
     minlp_integer_leaves = 1
     minlp_print_level = 1
     nlp_maximum_iterations = 1000
     objective_convergence_tolerance = 1.0×10^{-4}
     constraint_convergence_tolerance = 1.0×10^{-4}
7) Find a first candidate solution loading the model (24) in APMonitor using the IPOPT solver.
   - If the IPOPT solver cannot solve the problem because of the number of variables, change discretization in time N_t and return to step 2.
8) Find a candidate solution loading the model (24) with initial values of the previous solution in APMonitor using the APOPT solver.

9) Report the vector m for the lower level and the value Z_F for the upper level.
   - If you need more candidate solutions, go to step 8.

5.2. **Numerical results.** We present here the results of a problem that represents a shallow body of water built with ideal hydrological data and a simple geometry that was easy to replicate as shown in Figure 2. This assumes that there is an operating pollution firm in the zone already, which releases wastewater by a constant mass flow $m_2(t) = 100$ kg/m^{3}s at point c_2. We are interested in a wastewater treatment plant with discharge point $c_1 \in \Omega$, and we seek the amount of discharge at that point along the time $m_1(t)$ and the optimal penalty parameter of the fine function Z_F with the areas intended to protect, from an ecological point of view, by the EPA (A_L) and the treatment plant (A_F).

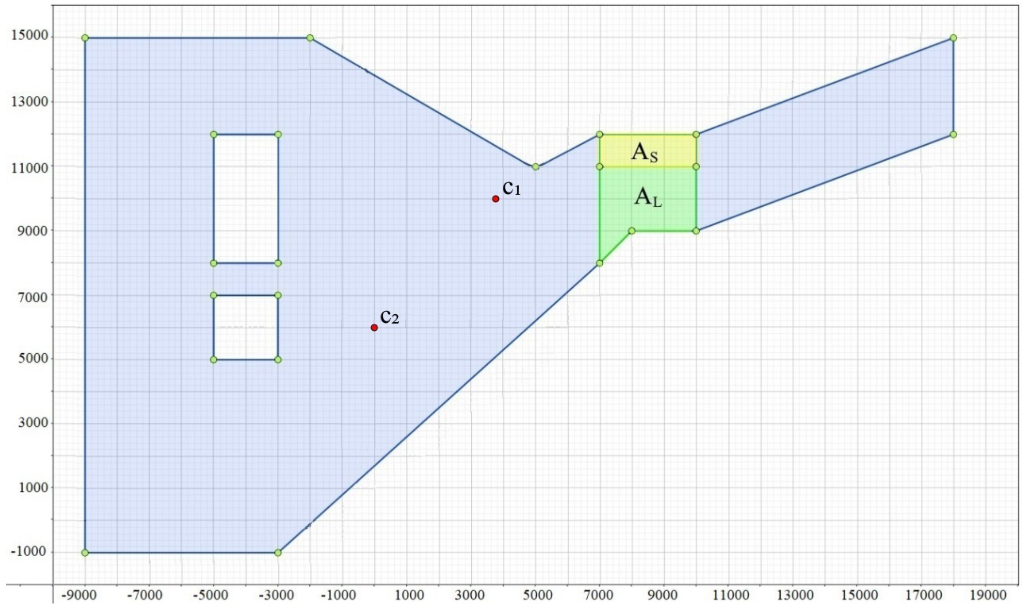

FIGURE 2. Domain Ω showing outfalls of a treatment plant c_1 and its protected area A_S, a polluting firm c_2 and the protected area of the EPA A_L

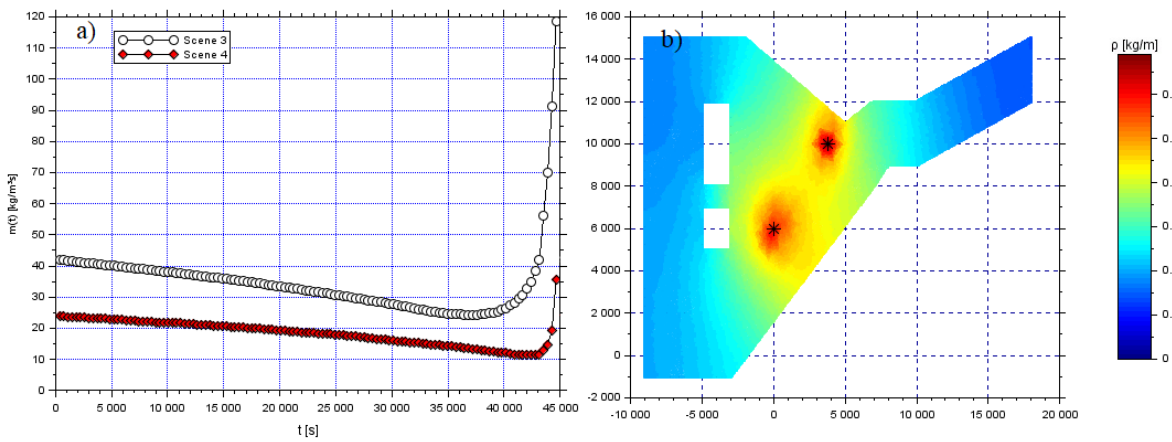

FIGURE 3. (color online) Mass flow m as a function of time t for a discharge point $b = (3750, 10000)$ in scenarios 3 (a) and 4 (a). Evolution of the concentration of FC estimated at the simulation termination of a controlled strategy in scenario 3 (b).

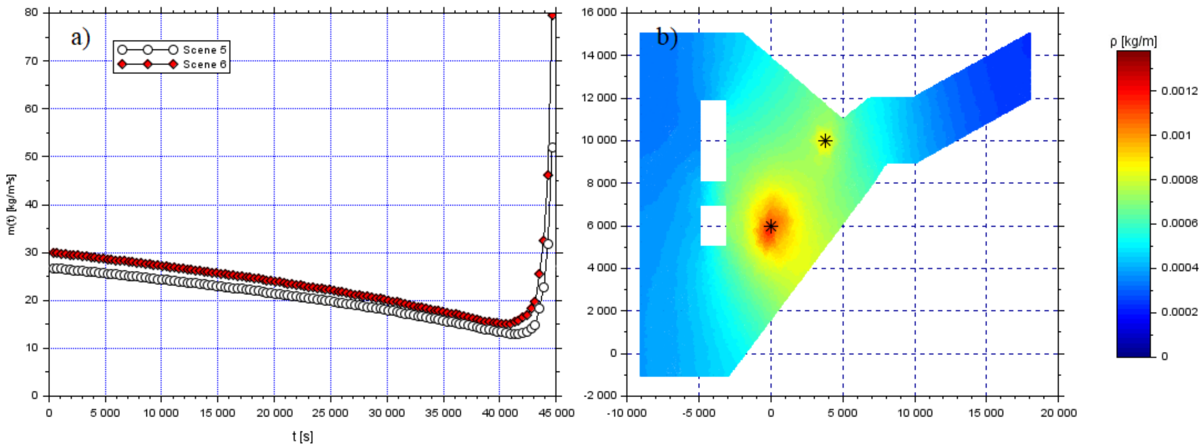

FIGURE 4. (color online) Mass flow m as a function of time t for a discharge point $b = (3750, 10000)$ in scenarios 5 (a) and 6 (a). Evolution of the concentration of FC estimated at the simulation termination of a controlled strategy in scenario 6 (b).

TABLE 1. Values of the mass flow of emissions discharged $m(t)$, and their numerical values of the functionals J_L (Leader) and J_F (Follower) using a bilevel optimization approach; the symbol † means a controlled variable for for testing purposes.

Scene	Z_F	$m(t)$ [kg/m^{3}s]	J_L	J_F
1	†3.83×10^4	†100	8.22×10^7	1.65×10^8
2	†3.83×10^4	†40	5.13×10^7	1.01×10^7
3	†3.83×10^4	Figure 3(a)	4.95×10^7	7.99×10^6
4	†8.00×10^7	Figure 3(a)	4.67×10^7	1.22×10^7
5	1.01×10^6	Figure 4(a)	4.65×10^7	1.06×10^7
6	5.11×10^6	Figure 4(a)	4.61×10^7	1.17×10^7

To show the results we present some scenes in Figure 3 and Figure 4 along with their numerical values of the functionals J_L (environmental impact) and J_F (economic costs) presented in Table 1.

The first two scenes are test runs that correspond to a random penalty parameter $Z_F = 3.82578 \times 10^4$ in an order of magnitude similar to the literature and discharge a constant mass flow $m(t) = 100$ kg/m^{3}s in scene 1 and a constant mass flow $m(t) = 40$ kg/m^{3}s in scene 2. Scenes 3 and 4 correspond to a fixed penalty parameter and find the optimal mass flow $m(t)$ with $Z_F = 3.82578 \times 10^4$ for scenario 3 and in scenario 4 penalty parameter $Z_F = 8.00 \times 10^7$ was chosen to be an order of magnitude greater than the optimal penalties obtained in scenarios 5 and 6; in Figure 3(a) we show the mass flow $m(t)$ of scenes 3 and 4 along with the FC concentrations at the end of the simulation of scene 3 in Figure 3(b). In scene 5 and 6, the penalty parameter Z_F is a manipulated variable from which values were obtained together with their respective optimal function $m(t)$ obtained by solving the BOP using the APOPT solver in APMonitor, in scenario 5 the initial values of Z_F and $m(t)$ are obtained from a previous run with the IPOPT solver in APMonitor; the scenario 6 corresponds to a scene with the lowest value of J_L obtained in different runs where the initial values of Z_F and $m(t)$ come from a previous solution obtained with the APOPT solver; in Figure 4(a) we show the mass flow $m(t)$ of scenes 5 and 6 along with the FC concentrations at the end of the simulation of scene 6 in Figure 4(b).

All scenarios were solved with the following parameters:
$c_1 = (3750, 10000)$: Outfall of treatment plant.
$c_2 = (0, 6000)$: Outfall of polluting firm.
$\vec{v}(s,t) = \vec{v}(x,y,t) = (0.050676, 0.050676)$ m/s, $\forall t \in [0,T]$: Velocity field.
$h(s,t) = h(x,y,t) = 37$ m, $\forall t \in [0,T]$: Height field.
$\beta = 2000$ m^2/s: Horizontal viscosity.
$k = 1.1510 \times 10^{-5}$/s: Kinetic coefficients.
$T = 12.4$ h $= 44640$ s: Tidal cycle.
$M_{ad} = \left[m^L, m^U\right] = 1 \leq m(t) \leq 150$, $\forall t \in [0,T]$.
$\sigma = 0.005$ kg/m^3: Threshold emission standard.
$J_C(x) = W_c \frac{100(150)^3}{x^3 - 3(150)x^2 + 3(150)^2 x}$: Cost of the purification process.
$J_I = 1240$: Inspection cost.
$Z_F^L = 0$ kg/m^3: Lower limit penalty parameter of emission fee.
$Z_F^U = 10^{10}$ kg/m^3: Upper limit penalty parameter of emission fee.
$Z_L = 13.2997 \times 10^{10}$ kg/m^3: Penalty parameter of ambient cost.
$W_c = 0.822$: Weight of the purification cost.

The choice of the penalty parameter of the emission fee point has a high impact on a treatment plant's management behavior. The first four scenarios serve as a reference to see the effects of the optimization on the quality of the treatments without considering the optimal location of the penalty parameter (see Figure 3). In the scenario 5 and 6, we obtain different candidate solutions that can be compared to each other to choose the most convenient solution. The increase in the emission fee penalty makes the plant reduce its emissions and that decreases the environmental impact on the body of water (see Figure 4 and Table 1).

6. **Conclusions.** We have formulated the wastewater regulation problem as a bilevel optimization problem that considers shallow bodies of water like estuaries, lakes, or coasts described by the Navier-Stokes equations where the damage caused by the emissions of the wastewater treatment plant has a non-linear behavior instead of linear behaviors of a river that have been worked on previously. The formulation gives us an interesting theoretical problem of some difficulties. Its reformulation of single-level means that one has to guarantee a local optimal single-level solution of the problem corresponding to a local optimal solution of the problem of bilevel. The state-system describing the emission concentration works as a pseudo third level and is described with the Navier-Stokes equation, which has no analytical solution in this case and defines the cost functions of the lower and upper levels. We developed a bilevel optimization problem and discretization techniques that can find numerical solutions to the location of wastewaters outfall problems. The future research includes deriving a bilevel optimal control problem using the lower level optimal value function method in the single level-reformulation and developing a maximum principle for this problem.

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