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Application of the optimal control theory to the wastewater elimination problem

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Abstract. The main goal of this paper is to show some applications of the optimal control theory to the wastewater elimination problem. Firstly, we deal with the numerical simulation of a given situation. We present a suitable mathematical model, propose a method to solve it and show the numerical results for a realistic situation in the *ría of Arousa* (Spain). Secondly, in the same framework of wastewater elimination problem, we pose two economic-environmental problems which can be formulated as constrained optimal control problems. For each of them, we give a theoretical analysis, introduce numerical methods and show results for real situations.

Aplicaciones de la teoría de control óptimo al problema de la eliminación de aguas residuales

Resumen. El principal objetivo de este trabajo es mostrar algunas de las aplicaciones de la teoría de control óptimo a problemas relacionados con la eliminación de aguas residuales. Como primer paso se aborda el problema de la simulación numérica de una situación dada, presentando un modelo matemático adecuado, señalando como resolverlo numéricamente y mostrando los resultados obtenidos en una situación realista planteada en la *ría de Arousa* (España). A continuación, en el marco de la problemática de eliminación de aguas residuales, se plantean dos problemas económico-ecológicos que se formulan, a partir del modelo anterior, como problemas de control óptimo con restricciones. Se analizan teóricamente, se indica como pueden resolverse numéricamente y se muestran los resultados obtenidos en una situación realista.

1. Introduction

The wastewater elimination problem arise from the growing industrialization and population explosion around urban areas. Wastewater, just like any other waste, has increased at cities in last years and it has became a very important problem that has not been completely solved yet. In coastal areas, a widespread solution is to discharge wastewater into the sea. In order to do it, a treatment system must be constructed. It consists of some purifying plants: each of them collects the sewage from different urban areas, treats it with chemical or biological methods and, finally, discharges it into the sea by means of a submarine outfall (see fig. 1).

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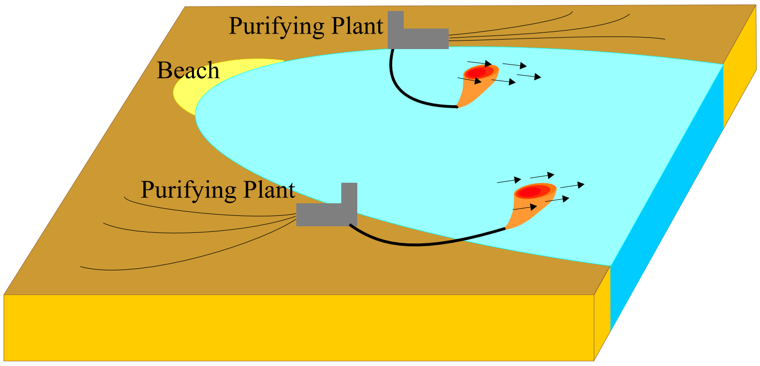

Figure 1. A wastewater treatment system.

The construction of this system is very expensive and, moreover, the environmental consequences could be very dangerous if the discharges are not carried out carefully. Thus a study of the environmental impact must be done in a previous stage. In this study, mathematical modelling can be very useful and so a first mathematical problem arises: the numerical simulation of a hypothetical situation. We have to compute the pollutant concentration in the domain where we are going to discharge wastewater through submarine outfalls.

A more interesting problem than simulating a given situation is designing an optimal one. This is the case, for example, of determining the optimal location of submarine outfalls or the pollution reduction to be done in each purifying plant in order to minimize the depuration cost of the whole system while guaranteeing the water quality in certain *sensible areas* as beaches, fish nurseries, etc.

The main goal of this paper is to show some results obtained by the authors along the last years. The outline of the paper is as follows. The next section is devoted to simulate a hypothetical situation: we present a mathematical model governing the pollutant concentration in a shallow water domain where wastewater are discharged through submarine outfalls. Then we propose a numerical method to solve it and show numerical results obtained for a hypothetical situation posed in the *ría of Arousa* (Spain). Next, sections 3 and 4 are devoted to study the two above mentioned problems related to the design of optimal situations. For each of them, we introduce a mathematical formulation, give theoretical analysis, and propose numerical methods. Finally, some results obtained in a realistic situation are shown.

2. Wastewater discharges. Numerical simulation

We consider a domain Ω, with boundary Γ, occupied by shallow water. It can be a *ría*, an estuary or a lake. Polluting wastewater are discharged through N_E submarine outfalls located at points $b_j \in \Omega$ and connected to their respective purifying plants located at points $a_j \in \Gamma$ (see fig. 2). Moreover, we assume that there exist several areas $A_i \subset \Omega, \quad i = 1, \dots, N_Z$ in the domain representing fisheries, beaches or marine recreation where it is necessary to guarantee the water quality with pollution levels lower than some allowed threshold levels.

Firstly, in order to simulate the water quality in Ω, we have to choose some indicators of pollution levels. Two of the most important (especially in the case of domestic discharges) are the *Dissolved Oxygen* (DO) and the organic matter, which can be measured in terms of the need of oxygen to decompose it, the so-called *Biochemical Oxygen Demand* (BOD). If the pollution level is not too high the BOD can be satisfied by the DO. However, if the organic matter increases beyond a maximum value the DO is not enough for its decomposition, leading to important modifications (anaerobic processes) in the ecosystem. To avoid them a threshold value of BOD may not be exceeded and a minimum level of DO must be guaranteed.

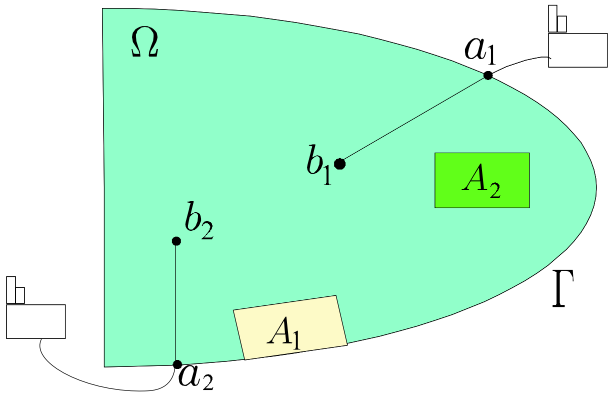

Figure 2. Domain Ω.

2.1. Mathematical model

The evolution of the BOD and the DO in the domain $\Omega \subset \mathbb{R}^2$ is governed by a system of partial differential equations (cf. [5]). Let us denote by $\rho_1(x,t)$ and $\rho_2(x,t)$ the concentrations of BOD and DO at point $x \in \Omega$ and at time $t \in [0,T]$, respectively. Then these concentrations are obtained as the solution of the following two initial-boundary value problems:

$$\left.\begin{array}{ll}
\dfrac{\partial \rho_1}{\partial t} + \vec{u}.\nabla \rho_1 - \beta_1 \Delta \rho_1 = -\kappa_1 \rho_1 + \dfrac{1}{h}\displaystyle\sum_{j=1}^{N_E} m_j \delta(x-b_j) & \text{in } \Omega \times (0,T) \\
\dfrac{\partial \rho_1}{\partial n} = 0 & \text{on } \Gamma \times (0,T) \\
\rho_1(x,0) = \rho_{10}(x) & \text{in } \Omega \\
\dfrac{\partial \rho_2}{\partial t} + \vec{u}.\nabla \rho_2 - \beta_2 \Delta \rho_2 = -\kappa_1 \rho_1 + \dfrac{1}{h}\kappa_2(d_s - \rho_2) & \text{in } \Omega \times (0,T) \\
\dfrac{\partial \rho_2}{\partial n} = 0 & \text{on } \Gamma \times (0,T) \\
\rho_2(x,0) = \rho_{20}(x) & \text{in } \Omega
\end{array}\right\} \qquad (1)$$

where $m_j(t)$ is the mass flow rate of BOD discharged at point b_j, $\delta(x-b_j)$ denotes the Dirac measure located at b_j and parameters $\beta_1 > 0$ and $\beta_2 >$ (horizontal viscosity coefficients), $\kappa_1 > 0$, κ_2 (kinetic coefficients related to BOD elimination and oxygen transfer through the surface, respectively) and d_s (oxygen saturation density) can be obtained from experimental measurements. The functions $h(x,t)$ and $\vec{u}(x,t)$ denote, respectively, the height and the mean horizontal velocity of the water; they may be previously obtained by solving the Saint-Venant (shallow water) equations:

$$\left.\begin{array}{ll}
\dfrac{\partial \eta}{\partial t} + \nabla.(h\vec{u}) = 0 & \text{in } \Omega \times (0,T) \\
\dfrac{\partial (hu_i)}{\partial t} + \displaystyle\sum_{j=1}^{2}\left(\frac{\partial (u_j h u_i)}{\partial x_j}\right) + gh\frac{\partial \eta}{\partial x_i} + \frac{\partial \rho_a}{\partial x_i} = F_i + \frac{1}{\rho}(\tau_w - \tau_f),\ i=1,2 & \text{in } \Omega \times (0,T) \\
(h\vec{u})\vec{\nu} = f & \text{on } \Gamma_0 \times (0,T) \\
h = \psi + H & \text{on } \Gamma_1 \times (0,T) \\
h(x,0) = h_0(x),\quad \vec{u}(x,0) = \vec{u}_0(x) & \text{in } \Omega
\end{array}\right\} \qquad (2)$$

where Γ_0 denotes the coast or effluent boundary, Γ_1 denotes the open sea boundary ($\Gamma = \Gamma_0 \cup \Gamma_1$), $\eta = h - H$ ($H(x)$ is the depth with respect to a reference level), and the other terms represent the effects of atmospheric pressure, wind stress and bottom friction (see for instance [9] for further details).

2.2. Numerical resolution

The numerical resolution of the previous model consists of two steps. First of all, we have to solve the Saint-Venant equations (2) and then, when we know the velocity field, $\vec{u}(x,t)$, and the height of water, $h(x,t)$), we obtain the BOD and DO concentrations, $\rho_1(x,t)$ and $\rho_2(x,t)$, by solving the system (1).
In the present paper, the Saint-Venant equations are solved by using an implicit in time numerical scheme and Raviart-Thomas finite elements for the space discretization (see [9]). For the system (1) we use a method which combines characteristics for time discretization with finite elements for space discretization. Further details can be found in [1] or [2] where numerical convergence is proved.

2.3. Numerical results

The model (1)-(2) has been used to simulate the velocity field and the BOD-DO concentrations in several *rías* of Galicia (Spain). In this section we present the numerical results obtained in the *ría* of Arousa during a complete tidal cycle for two different wind conditions. We assume wind velocity is 22 m/s and consider two opposite directions: SW and NE. The sensibility of the model can be assessed from the figures 3, 4 and 5. They show, respectively, velocity field, BOD concentration and DO concentration at middle-hight tide for the two different wind directions. We observe that the NE direction reduces the tidal velocity of the water at this moment (specially in the shallow zones). This implies that the mouth of the *ría* is less polluted with NE wind than with SW wind which is rather intuitive.

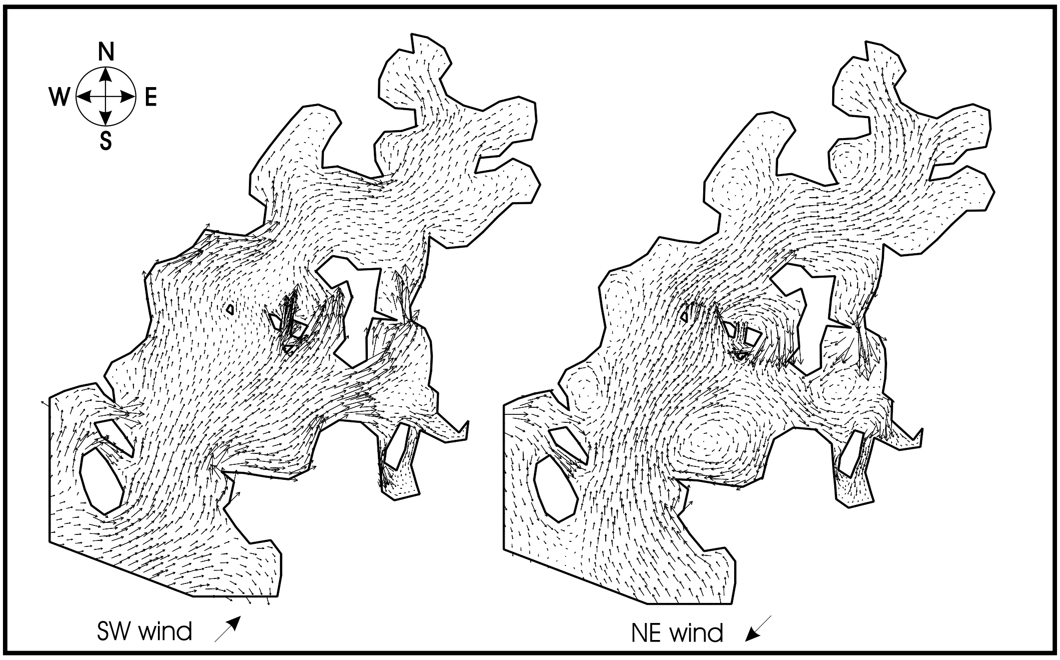

Figure 3. Velocity field at middle-hight tide (*ría* of Arousa).

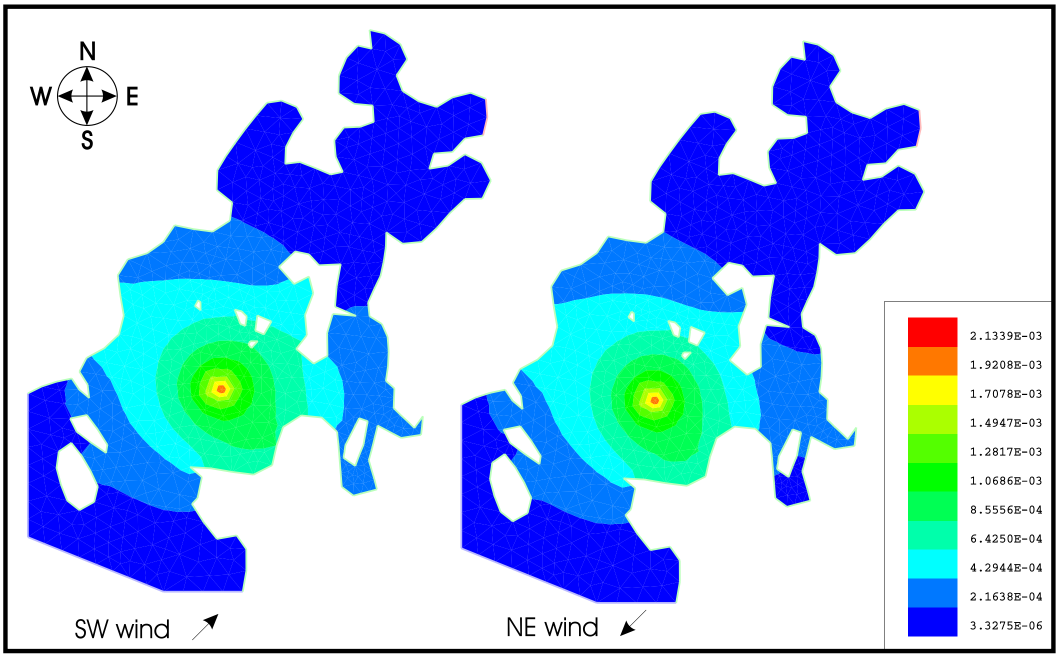

Figure 4. BOD concentration at middle-hight tide (*ría* of Arousa).

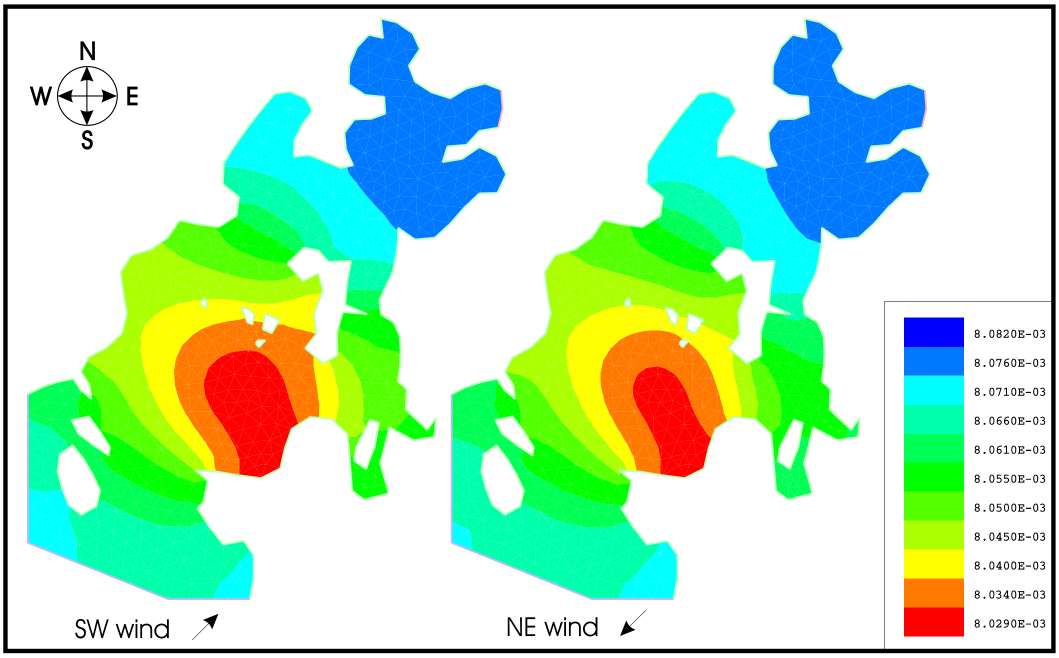

Figure 5. DO concentration at middle-hight tide (*ría* of Arousa).

3. Problem 1: Optimal management of a wastewater treatment system

In this section we are going to study an optimal control problem related to the management of a wastewater treatment system. We recall that we have a domain occupied by shallow water where polluting wastewater are discharged through N_E submarine outfalls (at this moment we suppose that these outfalls are already located at points $b_j \in \Omega$). Moreover, there exist several *sensible areas*, $A_i \in \Omega$, in the domain, where it is necessary to guarantee the water quality with pollution levels lower than an allowed threshold. We suppose that wastewater arrive to the purifying plants with a certain BOD concentration. Before discharging them into the sea, its BOD concentration can be reduced in the plants by different biological or biochemical treatments. From the ecological point of view the depuration in each plant must be as high as possible but, from the economical point of view, there is a cost proportional to the realized depuration. Then, the optimal management problem is to determine the depuration at each plant along the time, in such a way that the global depuration cost is minimized and the above constraints on the water quality are satisfied.

3.1. Mathematical formulation

In order to formulate this problem we need to take into account some issues. Firstly, if $\bar{m}_j$ denotes the BOD of wastewater arriving to the $j-th$ plant and $\underline{m}_j$ is the BOD corresponding to the maximum depuration at that plant, then determining the depuration at the $j-th$ plant is equivalent to finding the mass flow rate of BOD, $m_j(t)$, discharged through the corresponding outfall. We assume they satisfy the constraints

$$\underline{m}_j \leq m_j(t) \leq \bar{m}_j \quad j = 1, 2, \ldots, N_E. \tag{3}$$

Secondly, if we take BOD and DO as indicators of the water quality, then the environmental constraints on it can be written as follows (see section 2):

$$\left\{ \begin{array}{ll} \rho_{1|A_i} \leq \sigma_i & i = 1, \ldots, N_Z \\ \rho_{2|A_i} \geq \zeta_i & i = 1, \ldots, N_Z. \end{array} \right. \tag{4}$$

Finally, we suppose that the cost of the depuration process at the $j-th$ plant is known and it is a strictly convex C^2-function of the BOD discharged through the corresponding outfall. Hence, if f_j denotes the cost function at $j-th$ plant, the cost of the whole depuration is given by,

$$J_1(m) = \sum_{j=1}^{N_E} \int_0^T f_j\left(m_j(t)\right) dt. \tag{5}$$

According to this, the optimal management problem $(\mathcal{P}_1)$ consists of finding the functions $m_j(t), \quad j = 1, \ldots, N_E$, minimizing the cost function (5) in such a way that the corresponding state of the system given by (1) satisfies the constraints (3) and (4).

This is an optimal control problem with pointwise state constraints and with pointwise control. From the theoretical point of view the main difficulties are first the fact that the source term of the state system includes Radon measures and second the presence of pointwise state constraints. Numerically, difficulties arise from the high dimension of the discrete control space and the high number of discrete constraints related to time and space discretization.

3.2. Theoretical Analysis

First of all, we state the existence and uniqueness of solution for the state system.

Definition 1 *Given* $r,\ s \in [1,2)$, $\dfrac{2}{r}+\dfrac{2}{s} > 3$, *we say that* $\rho = (\rho_1, \rho_2) \in [L^r(0,T;W^{1,s}(\Omega))]^2$, *is a solution of the system (1) if for all* $\Phi = (\Phi_1, \Phi_2) \in [L^2(0,T;H^2(\Omega)) \cap H^1(0,T;L^2(\Omega))]^2 \cap [C^1(\bar{\Omega}\times[0,T]]^2$ *such that* $\Phi(.,T) = 0$, *the following equality holds:*

$$\begin{aligned}
&\int_0^T \int_\Omega \{-\frac{\partial \Phi_1}{\partial t}\rho_1 - \frac{\partial \Phi_2}{\partial t}\rho_2 + \beta_1 \nabla\Phi_1.\nabla\rho_1 + \beta_2\nabla\Phi_2.\nabla\rho_2 + \Phi_1 \vec{u}.\nabla\rho_1 \\
&\qquad + \Phi_2\vec{u}.\nabla\rho_2 + \kappa_1\Phi_1\rho_1 + \kappa_1\Phi_2\rho_1 + \frac{1}{h(x,t)}\kappa_2\Phi_2\rho_2)\}\, dx\, dt \\
&\qquad = \sum_{j=1}^{N_E}\int_0^T \frac{1}{h(P_j,t)}\Phi_1(P_j,t)m_j(t)\, dt \\
&\qquad + \int_0^T \int_\Omega \frac{1}{h(x,t)}\kappa_2 d_s \Phi_2(x,t)\, dx\, dt + \int_\Omega \Phi_2(x,0)\rho_{20}(x)\, dx.
\end{aligned} \tag{6}$$

Let $\mathcal{A}$ be the operator defined by

$$\begin{aligned}
\langle \mathcal{A}(w_1,w_2),(z_1,z_2)\rangle &= \int_\Omega (-\beta_1\Delta w_1 z_1 - \beta_2 \Delta w_2 z_2 \\
&\quad + \vec{u}.\nabla w_1 z_1 + \vec{u}.\nabla w_2 z_2 + \kappa_1 w_1 z_1 + \kappa_1 w_1 z_2 + \frac{1}{h}\kappa_2 w_2 z_2)\, dx,
\end{aligned}$$

for $(w_1,w_2),(z_1,z_2)$ such that the previous expression makes sense. Then we have the following:

Theorem 1 *There exists a unique pair*

$$\rho = (\rho_1,\rho_2) \in [L^r(0,T;W^{1,s}(\Omega))]^2 \cap [L^2(0,T;L^2(\Omega))]^2,$$

with

$$\frac{\partial\rho}{\partial t} = (\frac{\partial\rho_1}{\partial t}, \frac{\partial\rho_2}{\partial t}) \in [L^r(0,T;(W^{1,s'}(\Omega))')]^2$$

for all $r,\ s \in [1,2)$, $\dfrac{2}{r}+\dfrac{2}{s} > 3$, *such that* ρ *is solution of (6) and verifies*

$$\begin{aligned}
\int_0^T \langle -\frac{\partial\Phi}{\partial t} + \mathcal{A}^*(\Phi), \rho\rangle dt &= \sum_{j=1}^{N_E}\int_0^T \frac{1}{h(P_j,t)}\Phi_1(P_j,t)m_j(t)\, dt \\
&+ \int_0^T\int_\Omega \frac{1}{h(x,t)}\kappa_2 d_s\Phi_2(x,t)\, dx\, dt + \int_\Omega \Phi_2(x,0)\rho_{20}(x)\, dx,
\end{aligned} \tag{7}$$

for all $\Phi = (\Phi_1,\Phi_2) \in \mathcal{B}$, *where*

$$\begin{aligned}
\mathcal{B} = \{\Phi = (\Phi_1,\Phi_2) &\in [L^2(0,T;H^2(\Omega)) \cap H^1(0,T;L^2(\Omega))]^2 \ : \\
-\frac{\partial\Phi}{\partial t} + \mathcal{A}^*(\Phi) &\in [L^2(0,T;L^2(\Omega))]^2, \quad \frac{\partial\Phi}{\partial n_{\mathcal{A}^*}}_{|\Gamma\times(0,T)} = 0, \quad \Phi(.,T) = 0\}.
\end{aligned}$$

Furthermore, there exist constants $C_k,\ k = 1,\ldots,6$, *depending only on data, such that*

$$||\rho||_{[L^r(0,T;W^{1,s}(\Omega))]^2} \leq C_1 \sum_{i=1}^{N_E} ||m_i||_{L^\infty(0,T)} + C_2||\rho_{20}||_{C(\bar{\Omega})} + C_3\, d_s. \tag{8}$$

and

$$||\rho||_{[L^2(0,T;L^2(\Omega))]^2} \leq C_4 \sum_{i=1}^{N_E} ||m_i||_{L^\infty(0,T)} + C_5||\rho_{20}||_{C(\bar{\Omega})} + C_6\, d_s. \quad \square \tag{9}$$

The proof of this theorem can be seen in [11], as well as the following regularity and continuity results.

Lemma 1 *Functions* ρ_1 *and* ρ_2 *are continuous in* $\bar{A}_i \times [0,T]$, $\forall\, i = 1,\dots,N_Z$. $\square$

Lemma 2 *There exist constants* $\hat{C}_1, \hat{C}_2, \hat{C}_3$ *such that*

$$\|\rho\|_{[C(\cup_{i=1}^{N_Z}\bar{A}_i\times[0,T])]^2} \le \hat{C}_1 \sum_{i=1}^{N_E} \|m_i\|_{L^\infty(0,T)} + \hat{C}_2\, \|\rho_{20}\|_{C(\bar{\Omega})} + \hat{C}_3\, d_s. \quad \square$$

Concerning existence of solution to the optimal control problem $(\mathcal{P}_1)$, we define

$$M_{ad} = \{m \in (L^\infty(0,T))^{N_E} \ : \ 0 < \underline{m}_j \le m_j(t) \le \overline{m}_j \ \text{ a.e. in } (0,T),\ j = 1,\dots,N_E\}.$$

We have the following result:

Theorem 2 *If there exists a feasible control* $\tilde{m} \in M_{ad}$ *such that the corresponding state* $\tilde{\rho}$ *satisfies the constraints*

$$\begin{aligned} \tilde{\rho_1}_{|A_i\times(0,T)} &\le \sigma_i, \quad i = 1,\dots,N_Z,\\ \tilde{\rho_2}_{|A_i\times(0,T)} &\ge \zeta_i, \quad i = 1,\dots,N_Z, \end{aligned}$$

then the optimal control problem $(\mathcal{P}_1)$ *has a unique solution.* $\square$

Finally, in order to write an optimality system, we define

$$F_1 : m \in (L^\infty(0,T))^{N_E} \longrightarrow F_1(m) = {\rho_1}_{|\cup_{i=1}^{N_Z}\bar{A}_i\times[0,T]} \in C(\cup_{i=1}^{N_Z}\bar{A}_i \times [0,T]),$$

$$F_2 : m \in (L^\infty(0,T))^{N_E} \longrightarrow F_2(m) = {\rho_2}_{|\cup_{i=1}^{N_Z}\bar{A}_i\times[0,T]} \in C(\cup_{i=1}^{N_Z}\bar{A}_i \times [0,T]),$$

and state their Gateaux derivability.

Lemma 3 *The mappings* F_1 *y* F_2 *are Gateaux derivable. Moreover*

$$DF_1(m)(n) = {\omega_1}_{|\cup_{i=1}^{N_Z}\bar{A}_i\times[0,T]},$$

$$DF_2(m)(n) = {\omega_2}_{|\cup_{i=1}^{N_Z}\bar{A}_i\times[0,T]},$$

where ω_1 *and* ω_2 *are the solution of the linearized system,*

$$\left.\begin{aligned} \frac{\partial \omega_1}{\partial t} + \vec{u}.\nabla\omega_1 - \beta_1\Delta\omega_1 &= -\kappa_1\omega_1 + \frac{1}{h}\sum_{j=1}^{N_E} n_j\delta(x-P_j) && \text{in } \Omega\times(0,T)\\ \frac{\partial \omega_1}{\partial n} &= 0 && \text{on } \Gamma\times(0,T)\\ \omega_1(x,0) &= 0 && \text{in } \Omega\\ \frac{\partial \omega_2}{\partial t} + \vec{u}.\nabla\omega_2 - \beta_2\Delta\omega_2 &= -\kappa_1\omega_1 - \frac{1}{h}\kappa_2\omega_2 && \text{in } \Omega\times(0,T)\\ \frac{\partial \omega_2}{\partial n} &= 0 && \text{on } \Gamma\times(0,T)\\ \omega_2(x,0) &= 0 && \text{in } \Omega \end{aligned}\right\} \tag{10}$$

From this Lemma one can obtain a first order optimality system satisfied by any solution of the optimal control problem. In order to express the optimality conditions in a simpler way we introduce functions p_1, p_2 solution (in the sense of Definition 2 below) of the following boundary value problem:

$$\left.\begin{array}{rl}
-\dfrac{\partial p_1}{\partial t} - \nabla.(\vec{u}p_1) - \beta_1 \Delta p_1 + \kappa_1(p_1+p_2) = \mu_{1|\Omega\times(0,T)} & \text{in } \Omega\times(0,T) \\
\beta_1 \dfrac{\partial p_1}{\partial n} + \vec{u}.\vec{n}\, p_1 = 0 & \text{on } \Gamma\times(0,T) \\
p_1(x,T) = \mu_{1|\Omega\times\{T\}} & \text{in } \Omega \\
-\dfrac{\partial p_2}{\partial t} - \nabla.(\vec{u}p_2) - \beta_2 \Delta p_2 + \dfrac{1}{h}\kappa_2 p_2 = \mu_{2|\Omega\times(0,T)} & \text{in } \Omega\times(0,T) \\
\beta_2 \dfrac{\partial p_2}{\partial n} + \vec{u}.\vec{n}\, p_2 = 0 & \text{on } \Gamma\times(0,T) \\
p_2(x,T) = \mu_{2|\Omega\times\{T\}} & \text{in } \Omega
\end{array}\right\} \quad (11)$$

where μ_1, μ_2 are regular Borel measures in $\bar{\Omega}\times[0,T]$. The weak solution of the system (11) can be defined by transposition techniques (see [10]) in the following way:

Definition 2 *Given* $r,\ s \in [1,2),\ \dfrac{2}{r}+\dfrac{2}{s} > 3$, *we say that* $p = (p_1,p_2) \in [L^r(0,T;W^{1,s}(\Omega))]^2$ *is a solution of the system (11) if for all* $z = (z_1,z_2) \in [L^2(0,T;H^1(\Omega)) \cap C^1(\bar{\Omega}\times[0,T]]^2$ *such that* $z(.,0)=0$, *the following equality holds:*

$$\int_0^T \int_\Omega \{ \frac{\partial z_1}{\partial t}p_1 + \frac{\partial z_2}{\partial t}p_2 + \rho_1 \nabla z_1.\nabla p_1 + \rho_2 \nabla z_2.\nabla p_2 + \vec{u}.\nabla z_1 p_1 + \vec{u}.\nabla z_2 p_2$$
$$+\kappa_1 z_1 p_1 + \kappa_1 z_1 p_2 + \frac{1}{h(x,t)}\kappa_2 z_2 p_2)\}\, dx\, dt = \int_0^T \int_\Omega z_1 d\mu_1(x,t)$$
$$+ \int_0^T \int_\Omega z_1 d\mu_1(x,t) + \int_\Omega z_1(x,T) d\mu_{1T}(x) + \int_\Omega z_2(x,T) d\mu_{2T}(x).$$

Let us define the sets S_1 and S_2 by

$$S_1 = \{y \in C(\cup_{i=1}^{N_Z} \bar{A}_i \times [0,T]) :\ y(x,t) \le \sigma_j,\ \forall (x,t) \in \overline{A}_j \times [0,T],\ j=1,\ldots,N_Z\},$$
$$S_2 = \{\omega \in C(\cup_{i=1}^{N_Z} \bar{A}_i \times [0,T]) :\ \omega(x,t) \ge \zeta_j,\ \forall (x,t) \in \overline{A}_j \times [0,T],\ j=1,\ldots,N_Z\}.$$

We have the following

Theorem 3 *Let* $m \in M_{ad}$ *be an optimal control. Then there exist two functions* $\rho_1,\ \rho_2 \in L^r(0,T;W^{1,s}(\Omega)) \cap L^2(0,T;L^2(\Omega))$, *for all* $r,\ s \in [1,2),\ \dfrac{2}{r}+\dfrac{2}{s} > 3$, *which are solution of (1) and two functions* $p_1,\ p_2 \in L^r(0,T;W^{1,s}(\Omega))$ *solution of (11), where* $\mu_1,\ \mu_2$ *are two Borel measures with support in* $\cup_{i=1}^{N_Z} \bar{A}_i \times [0,T]$ *such that*

$$\mu_{i|\cup_{i=1}^{N_Z} \bar{A}_i \times [0,T]} \in \partial I_{S_i}(F_i(m)), \quad i=1,2, \tag{12}$$

and furthermore

$$\sum_{j=1}^{N_E} \left(\int_0^T f_j{}'(m_j(t))(n_j(t)-m_j(t))\, dt + \int_0^T \frac{1}{h(P_j,t)} p_1(P_j,t)(n_j(t)-m_j(t))\, dt \right) \ge 0, \quad \forall n \in M_{ad}. \tag{13}$$

Proof. See [11] ■

3.3. Numerical solution

The numerical solution of the optimal control problem $(\mathcal{P}_1)$ requires a discretization in accordance with that of the state system. Thus from the numerical approximation of the state variables at grid points and time steps ($\rho_{ij}^n(x) \approx \rho_i(x_j, t_n)$) we define the function g_1 which put together the discretized state constraints:

$$\begin{array}{llll} g_1 : & \mathbb{R}^{N\times N_E} & \longrightarrow & \mathbb{R}^{N\times N_{VZ}} \mathrm{x} \mathbb{R}^{N\times N_{VZ}} \\ & m & \longrightarrow & g_1(m) = (\vec{\rho}_1 - \sigma, \zeta - \vec{\rho}_2), \end{array} \tag{14}$$

where $N \in \mathbb{N}$ is the number of time steps, $m = \{m_{jn}\}$ is the vector of all discharges at all time steps, N_{VZ} is the number of grid points in the protected areas and $\vec{\rho}_i$ is the vector of values of ρ_i at grid points included in the protected areas and for all time steps.

Moreover, because of the particular shape of the functions f_j the constraints $m_j(t) \leq \bar{m}_j$ can be suppressed. Then, denoting $\underline{m} = \{\{\underline{m}_j\}_{n=1}^N\}_{j=1}^{N_E}$, the function g_2 collects the discretized control constraints:

$$\begin{array}{llll} g_2 : & \mathbb{R}^{N\times N_E} & \longrightarrow & \mathbb{R}^{N\times N_E} \\ & m & \longrightarrow & g_2(m) = \underline{m} - m. \end{array} \tag{15}$$

Finally, the cost function is approximated by using a quadrature formula:

$$\begin{array}{llll} \hat{J}_1 : & \mathbb{R}^{N\times N_E} & \longrightarrow & \mathbb{R} \\ & m & \longrightarrow & \hat{J}_1(m) = \dfrac{T}{N} \displaystyle\sum_{j=1}^{N_E} \sum_{n=1}^{N} Q_{jn} f_j(m_{jn}), \end{array} \tag{16}$$

where m_{jn} is the mass flow rate of BOD discharged at b_j at time t_n and Q_{jn} are the weights of the quadrature formula.

Then the optimal control problem $(\mathcal{P}_1)$ is approximated by the following *discrete* optimization problem:

$$(\mathcal{P}_{1D}) \left\{ \begin{array}{l} \displaystyle\min_{m\in\mathbb{R}^{N\times N_E}} \quad \hat{J}_1(m) \\ \\ \text{such that } \; g_i(m) \leq 0 \quad i = 1, 2. \end{array} \right.$$

Now this problem can be solved by different numerical methods (we refer to [12] for a numerical resolution of $(\mathcal{P}_{1D})$ by using a succesive quadratic programming algorithm and an admissible points method).

3.4. Numerical results

In this section we present the numerical results obtained when solving the previous problem for a realistic situation posed in the *ría* of Arousa during a complete tidal cycle (T=12.4h). We have taken four submarine outfalls and nine protected areas (see Fig. 6), and we have considered the same constraints on the nine zones.

The cost function is the same at every purifying plant and it is given in Figure 9. We assume that pollutant concentration of wastewater arriving to the purifying plant is 150 $\mathrm{kg/m^3}$ so the depuration cost above this value is constant.

The values of the optimal discharges can be seen in Figure 8. For these discharges, Figures 6 and 7 show, respectively, the BOD and DO concentration at high tide, at the end of the tidal cycle that we have simulated. The constraints are satisfied everywhere in the protected areas and the saturation takes place for the BOD concentration at several points.

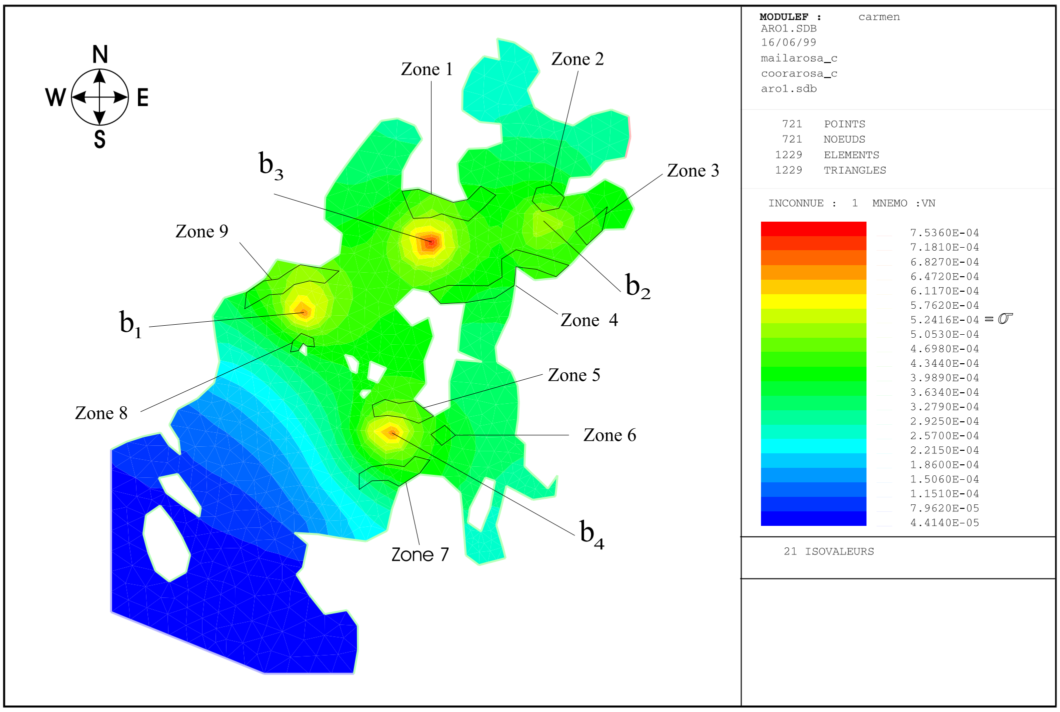

Figure 6. BOD concentration at high tide corresponding to the optimal discharges (*ría* of Arousa).

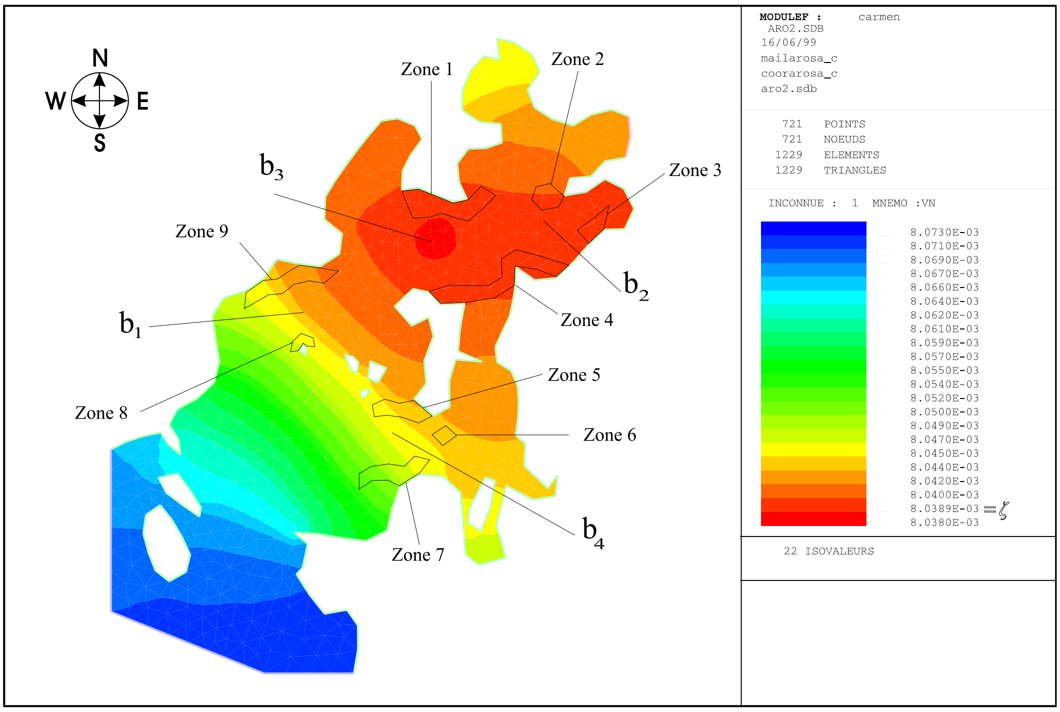

Figure 7. DO concentration at high tide corresponding to the optimal discharges (*ría* of Arousa).

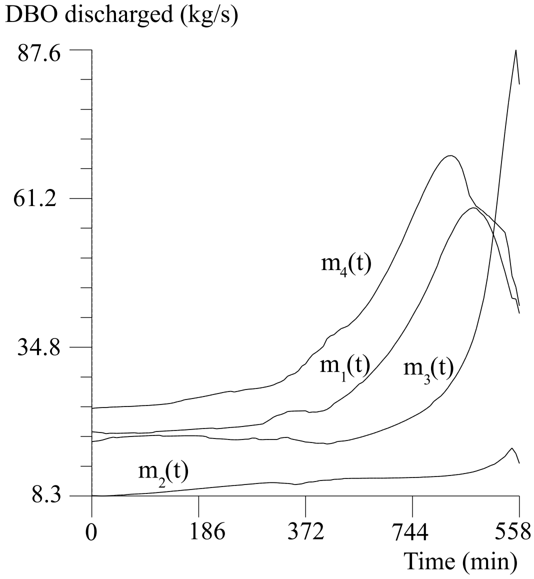

Figure 8. Optimal discharges.

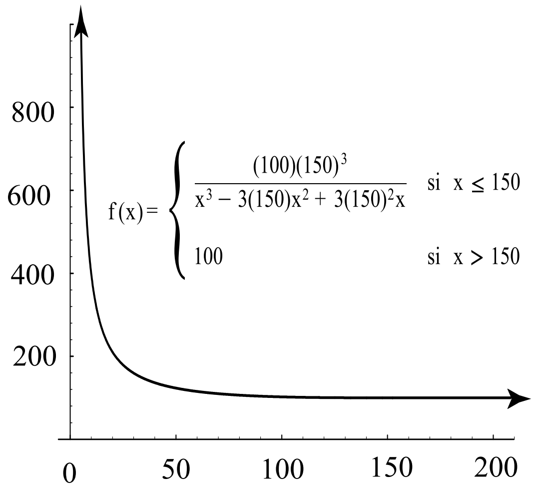

Figure 9. Cost function.

4. Problem 2: Optimal location of wastewater outfalls

The second problem is connected with the optimal design of a wastewater treatment system. Particulary, it consists of finding the optimal location of the submarine outfalls.

We consider a similar situation to the previous one: a domain occupied by shallow water where we are going to discharge polluting wastewater through submarine outfalls and where there exist several *sensible areas* in which we have to guarantee the water quality in terms of BOD and DO. Moreover, we also suppose that there are N_E purifying plants (located at points $a_j \in \Gamma$) but, unlike the previous problem, we now assume that the depuration in every plant is fixed (the functions $m_j(t)$ are known beforehand) and our goal is to determine the points b_j where wastewater will be discharged. These points must be determined in order to minimize the construction cost of the submarine outfalls while guaranteeing the water quality at the sensible areas.

4.1. Mathematical formulation

The constraints on the water quality are given in (4). Moreover, taking into account technological limitations, the j-th outfall must be placed in a suitable region U_j, where $U_j \subset \Omega \backslash \cup_{i=1}^{N_Z} \bar{A}_i$ is a compact convex polyhedral set representing all the admissible points where outfalls can be located. Thus, the optimal locations must verify $b_j \in U_j,\ \forall j = 1, \ldots, N_E$. If we define $U_{ad} = \Pi_{j=1}^{N_E} U_j$, this constraint can be written in the simpler way

$$b \in U_{ad}. \tag{17}$$

Finally, we suppose that the construction cost of the j-outfall depends on the distance between the purifying plant (located at point $a_j \in \Gamma$) and the point of discharge, $b_j \in \Omega$. Hence we consider that the global cost of the system is given by

$$J_2(b) = \sum_{j=1}^{N_E} \frac{1}{2} ||b_j - a_j||^2. \tag{18}$$

Then the problem of optimal design, denoted by $(\mathcal{P}_2)$, consists of finding the points $b_j,\ j = 1,\dots,N_E$ minimizing the cost function (18) under the constraints (4) and (17).

This is a control problem with quadratic cost but with non-convex pointwise state constraints which makes difficult its analysis and resolution. A related steady state problem has been previously studied in [8]

4.2. Theoretical Analysis

We consider the mapping

$$\bar{F} : b \in U_{ad} \longrightarrow \bar{F}(b) = \rho_{|\cup_{i=1}^{N_Z} \bar{A}_i \times [0,T]} \in [C(\cup_{i=1}^{N_Z} \bar{A}_i \times [0,T])]^2.$$

For the sake of simplicity we denote $\bar{F}_1(b) = \rho_{1|\cup_{i=1}^{N_Z} \bar{A}_i \times [0,T]}$ and $\bar{F}_2(b) = \rho_{2|\cup_{i=1}^{N_Z} \bar{A}_i \times [0,T]}$. Then, as a consequence of the regularity of the Green matrix $G = (G_{ln})_{1\le l,n\le 2}$ of the state system, the following regularity result can be obtained (see [3]):

Theorem 4 *The mappings $\bar{F}_1$ and $\bar{F}_2$ are continuous and Gâteaux differentiable.* □

Now, by using minimizing sequences we have the following existence result:

Theorem 5 *If there exists a feasible control $\tilde{b} \in U_{ad}$ such that the corresponding state $\tilde{\rho}$ satisfies the constraints:*

$$\begin{aligned} \tilde{\rho_1}_{|\bar{A}_i \times [0,T]} &\le \sigma_i, \qquad \forall i = 1,\dots,N_Z \\ \tilde{\rho_2}_{|\bar{A}_i \times [0,T]} &\ge \zeta_i, \qquad \forall i = 1,\dots,N_Z \end{aligned}$$

then the optimal control problem has, at least, one solution. □

Finally, by using a mollifier sequence for the Dirac measure we obtain a first order optimality system satisfied by the solutions of the optimal control problem. Indeed, by using the functions p_1, p_2 solution of the problem (11) we have the following result (see [3]):

Theorem 6 *Let $b \in U_{ad}$ be an optimal control. Then, there exist two functions $\rho_1,\ \rho_2 \in L^r(0,T;W^{1,s}(\Omega)) \cap L^2(0,T;L^2(\Omega))$, for all $r,\ s \in [1,2)$, $\dfrac{2}{r} + \dfrac{2}{s} > 3$, solving (1), two Borel measures $\mu_1,\ \mu_2$ with support in $\cup_{i=1}^{N_Z} \bar{A}_i \times [0,T]$, two functions $p_1,\ p_2 \in L^r(0,T;W^{1,s}(\Omega))$ solving (11) and a non-negative constant λ such that*

$$\mu_{k|\cup_{i=1}^{N_Z} \bar{A}_i \times [0,T]} \in \partial I_{S_k}(F_k(b)), \quad k = 1,2, \tag{19}$$

$$\lambda + \|\mu_1\| + \|\mu_2\| > 0, \tag{20}$$

and the following relation holds:

$$\sum_{j=1}^{N_E} \{\lambda \langle b_j - a_j, c_j - b_j\rangle + \int_0^T m_j(t) \langle \nabla(\frac{1}{h(b_j,t)} p_1(b_j,t)), c_j - b_j\rangle \, dt\} \ge 0,\ \forall c \in U_{ad}. \quad \square \tag{21}$$

4.3. Numerical resolution

Now, in order to solve the problem $(\mathcal{P}_2)$, we introduce a discretization of the control problem in accordance with the one made for the state system. Firstly, the function collecting the discretized state constraints is denoted by $\bar{g}_1$,

$$\begin{array}{llll} \bar{g}_1 : & \mathbb{R}^{2\times N_E} & \longrightarrow & \mathbb{R}^{N\times N_{VZ}} \mathrm{x} \mathbb{R}^{N\times N_{VZ}} \\ & b & \longrightarrow & \bar{g}_1(b) = (\vec{\rho}_1 - \sigma,\ \zeta - \vec{\rho}_2). \end{array} \tag{22}$$

Secondly, we define a function $\bar{g}_2 : \mathbb{R}^{2\times N_E} \longrightarrow \mathbb{R}^r$ collecting all the linear constraints on the control which corresponds to the characterization of U_{ad}, i.e., $\bar{g}_2$ is such that $b \in U_{ad} \Leftrightarrow \bar{g}_2(b) \leq 0$.

Then the optimal control problem $(\mathcal{P}_2)$ is approximated by the following *discrete* optimization problem,

$$(\mathcal{P}_{2D}) \left\{ \begin{array}{l} \displaystyle\min_{b\in\mathbb{R}^{2\times N_E}} \quad J_2(b) \\ \\ \text{such that } \ \bar{g}_i(b) \leq 0 \quad i = 1, 2. \end{array} \right.$$

This problem can be solved by the *admissible points method* used before for problem $(\mathcal{P}_{1D})$. However, in this case, the function collecting the state constraints, $\bar{g}_1$, is not affine. Now, in order to compute the matrix $\nabla\bar{g}_1(b)$ we need to approximate each Dirac measure $\delta(x - b_j) \in M(\Omega)$ by a suitable function $\delta_h(., b_j) \in L^2(\Omega)$ (see [1] for further details). Then we solve, for $j = 1, \ldots, N_E,\ k = 1, 2$, the approximated problems with measure data,

$$\left.\begin{array}{rll}
\dfrac{\partial z_1^{(j,k)}}{\partial t} + \vec{u}.\nabla z_1^{(j,k)} - \beta_1\Delta z_1^{(j,k)} + \kappa_1 z_1^{(j,k)} = -\dfrac{1}{h}m_j\dfrac{\partial\delta_h}{\partial x_k}(x, b_j) & & \text{in } \Omega\times(0,T) \\
\dfrac{\partial z_1^{(j,k)}}{\partial n} = 0 & & \text{on } \Gamma\times(0,T) \\
z_1^{(j,k)}(x, 0) = 0 & & \text{in } \Omega \\
\\
\dfrac{\partial z_2^{(j,k)}}{\partial t} + \vec{u}.\nabla z_2^{(j,k)} - \beta_2\Delta z_2^{(j,k)} + \kappa_1 z_1^{(j,k)} + \dfrac{1}{h}\kappa_2 z_2^{(j,k)} = 0 & & \text{in } \Omega\times(0,T) \\
\dfrac{\partial z_2^{(j,k)}}{\partial n} = 0 & & \text{on } \Gamma\times(0,T) \\
z_2^{(j,k)}(x, 0) = 0 & & \text{in } \Omega
\end{array}\right\}$$

and then we can show that

$$\frac{\partial\bar{g}_1(b)}{\partial b_j^k} = (z_1^{(j,k)}, -z_2^{(j,k)})^t$$

evaluated at all vertices in the protected areas and at all times.

The difficulties obtaining the gradient (and Hessian) of $\bar{g}_1(b)$, the essentially geometric nature of the original problem and the low dimension of the control invited us to use some other methods to solve the problem $(\mathcal{P}_{2D})$. In [4], three different algorithms are used to obtain the numerical solution of $(\mathcal{P}_{2D})$ namely an admissible points algorithm, the Nelder-Mead simplex method and a duality method. As we can see in that paper, due to the geometric nature of the problem, the three algorithms present a good performance, specially the Nelder-Mead method.

4.4. Numerical results

In this section we present the numerical results obtained when solving the problem $(\mathcal{P}_2)$ for a realistic situation posed in the *ría* of Vigo (Spain) during a complete tidal cycle. We have taken two purifying plants, located near the coast at points $a_1 = (0, 11000)$ and $a_2 = (6630, 7200)$, and two protected areas (see Fig. 10).

The state constraints for both protected areas corresponds to $\sigma_1 = 0.0002$, $\sigma_2 = 0.000135$, $\zeta_1 = 0.008067$, $\zeta_2 = 0.0000805$. The admissible set U_{ad} and the optimal locations $b_1 = (69, 10224)$ and $b_2 = (5535, 8278)$, given by the Nelder-Mead method can be seen in Figure 10. Moreover, this figure shows the BOD concentration at high tide, at the end of the tidal cycle that we have simulated.

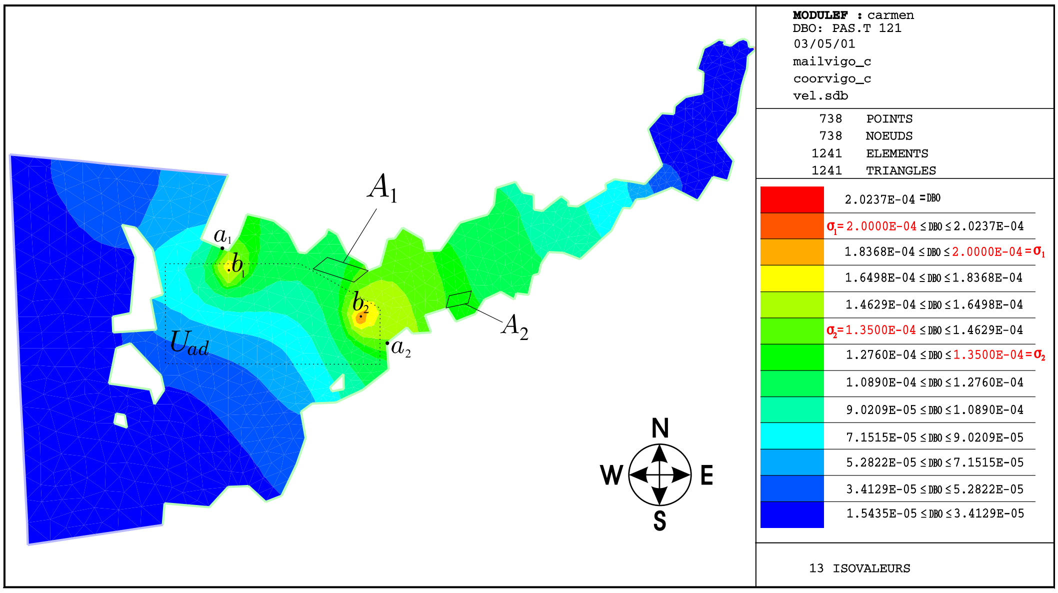

Figure 10. Optimal BOD concentration (hight tide, *ría* of Vigo).

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