ELSEVIER

Journal of Computational and Applied Mathematics 114 (2000) 67–79

JOURNAL OF COMPUTATIONAL AND APPLIED MATHEMATICS

A control problem arising in the process of waste water purification

A. Martínez[a,*,1], C. Rodríguez[b,1], M.E. Vázquez-Méndez[b,1]

[a] *Departamento de Matemática Aplicada, ETSI Telecomunicaciones, Universidad de Vigo, 36200 Vigo, Spain*

[b] *Departamento de Matemática Aplicada, Universidad de Santiago de Compostela, 15706 Santiago, Spain*

Received 10 December 1998; received in revised form 14 March 1999

Abstract

In this paper we state and solve an optimal control problem arisen from the management of the sewage disposal which is dumped into the sea through submarine outfalls. Firstly, we fix oxygen and amount of organic matter as water quality indicators and we state a partial differential equations model to simulate them in a domain occupied by shallow waters. Constraints about water quality and economic objectives lead us to a pointwise optimal control problem with state and control constraints. (The theoretical analysis of the problem has been developed by the authors in (Martinez et al., C. R. Acad. Sci. Paris, Serie I 328 (1999) 35.) (Martinez et al., Preprint, Dept. Matematica Aplicada, Univ. Santiago de Compostela, Spain, 1998.)). We deal with the problem by using time and space discretizations and we propose two algorithms for the numerical resolution of the discretized problem. Finally, we give numerical results obtained by applying the described techniques for a realistic problem posed in the *ría* of Vigo (Spain). © 2000 Elsevier Science B.V. All rights reserved.

Keywords: Pointwise control; Pointwise state constraints; Wastewater treatment; Constrained optimization

1. Introduction

We consider a domain $\Omega \subset \mathbb{R}^2$ occupied by shallow waters (see Fig. 1), for instance a *ría* or an estuary, and we suppose that the sewage is dumped into the domain Ω through N_E submarine outfalls, each of them located in a fixed point P_j in Ω and connected to a sewage farm. Moreover, we assumee the existence of N_Z areas in Ω (denoted by A_i), for example beaches or fish nurseries, where we need to guarantee the water quality with levels of pollution lower than maximum previously fixed values.

* Corresponding author.

E-mail address: aurea@dma.uvigo.es (A. Martínez)

[1] The research contained in this work was partially supported by Project XUGA20701A98 of Xunta de Galicia (Spain).

PII: S0377-0427(99)00289-7

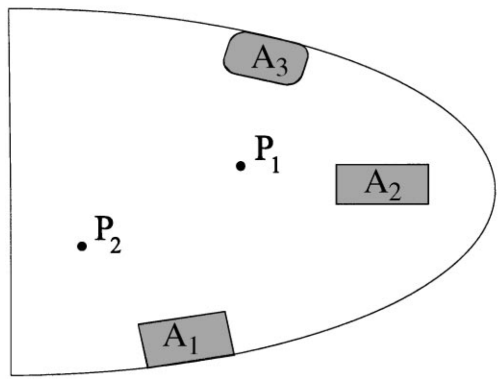

Fig. 1. Example of a possible domain Ω.

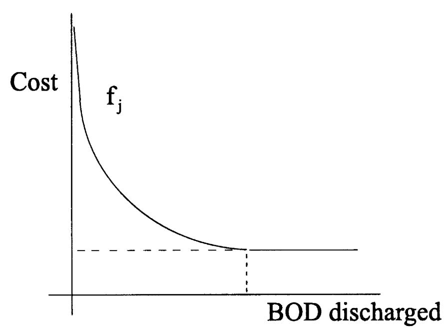

Fig. 2. Standard function $f_j(m)$ for the depuration cost.

In order to control those pollution levels several parameters can be used (dissolved oxygen, heavy metals, temperature, pH, radioactivity, etc.), which indicate the water quality and its capacity to hold aquatic life. Two of the most important (especially in the case of domestic discharges) are the *dissolved oxygen* (DO) and, directly related to it, the *biological oxygen demand* (BOD) which is required by bacteria to decompose the organic matter. As the pollution increases, the oxygen demand also increases and, as a result of this, the dissolved oxygen decreases. It damages marine life and causes that the organic matter decomposition continues by means of anaerobic processes, which do not use oxygen but produce sulphide of hydrogen and methane, both having a nauseating smell. To avoid this problem, we have to guarantee a minimum level σ_i of DO and a maximum level ζ_i of BOD in each region A_i to be protected. Consequently, any chemical and/or biological treatment of the waste water have to be made before the discharge.

We also assume that the depuration process cost in a particular sewage farm is known. This cost depends on the BOD discharge through the corresponding outfall, in such a way that in order to discharge a lower amount of BOD it is necessary to carry out a more intensive depuration, leading to a higher cost. Moreover, the complete purification of water is not possible and there is always a minimum cost, even with no depuration. Then, the function that represents the purification cost in the jth sewage farm has a shape as shown in Fig. 2.

Therefore, the optimal management problem consists of finding the discharges which reduce to the lowest level the total cost of the purification and guarantee the above mentioned constraints on the quality of the water.

2. Mathematical model: the continuous problem

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. [1,11]), which is a generalization of a previous one introduced by Streter and Phelps in 1928 to study pollution in the Ohio river. In this way, if the concentrations of BOD and DO at point $x \in \Omega$ and at time t are denoted by $\rho_1(x,t)$ and $\rho_2(x,t)$, respectively, then these concentrations are obtained as the solution of the following boundary value problem:

$$\begin{aligned}
&\frac{\partial \rho_1}{\partial t} + \boldsymbol{u}\nabla\rho_1 - \beta_1 \Delta\rho_1 = -\kappa_1\rho_1 + \frac{1}{h}\sum_{j=1}^{N_{\mathrm{E}}} m_j\delta(x-P_j) \quad \text{in } \Omega\times(0,T),\\
&\frac{\partial \rho_1}{\partial n} = 0 \quad \text{on } \Gamma\times(0,T),\\
&\rho_1(x,0) = \rho_{10}(x) \quad \text{in } \Omega,\\
&\frac{\partial \rho_2}{\partial t} + \boldsymbol{u}\nabla\rho_2 - \beta_2 \Delta\rho_2 = -\kappa_1\rho_1 + \frac{1}{h}\kappa_2(d_{\mathrm{s}}-\rho_2) \quad \text{in } \Omega\times(0,T),\\
&\frac{\partial \rho_2}{\partial n} = 0 \quad \text{on } \Gamma\times(0,T),\\
&\rho_2(x,0) = \rho_{20}(x) \quad \text{in } \Omega,
\end{aligned} \tag{1}$$

where Γ denotes the boundary of the domain Ω, $h(x,t)$ is the height of water and $\boldsymbol{u}(x,t)$ is the horizontal mean velocity. Both of them can be obtained as the solution of the Saint–Venant (shallow water) equations:

$$\begin{aligned}
&\frac{\partial \eta}{\partial t} + \nabla.(h\boldsymbol{u}) = 0,\\
&\frac{\partial (hu_i)}{\partial t} + \sum_{j=1}^{2}\left(\frac{\partial(u_j h u_i)}{\partial x_j}\right) + gh\frac{\partial \eta}{\partial x_i} + \frac{\partial \rho_a}{\partial x_i} = F_i + \frac{1}{\rho}(\tau_{\mathrm{w}} - \tau_{\mathrm{f}}), \quad i=1,2,
\end{aligned} \tag{2}$$

where $\eta = h - H$, for $H(x)$ a reference level, and the other terms represent the effects of atmospheric pressure, wind stress, bottom friction, etc. (see [2,3] for further details), $m_j(t)$, $j=1,\dots,N_{\mathrm{E}}$, is the mass flow rate of BOD discharged in P_j. This is the control of the problem, $\delta(x-P_j)$, $j=1,\dots,N_{\mathrm{E}}$, denotes the Dirac measure at point P_j.

The other parameter are experimentally known: β_1 and β_2 are horizontal viscosity coefficients, κ_1 is a kinetic parameter related to temperature, κ_2 is the interface transfer rate for oxygen and d_{s} is the oxygen saturation density in water.

Now, we assume that inside the domain Ω there are N_Z protected zones A_i where a maximum level of BOD and a minimum level of DO must be assured, that is

$$\rho_{1_{|A_i\times(0,T)}} \leqslant \sigma_i, \quad \forall i=1,\dots,N_Z, \tag{3}$$

$$\rho_{2_{|A_i\times(0,T)}} \geqslant \zeta_i, \quad \forall i=1,\dots,N_Z. \tag{4}$$

Moreover, taking into account technical limitations, the discharges of BOD must be larger than a certain value $\underline{m}$:

$$m_j(t) \geqslant \underline{m} \geqslant 0, \quad \forall j=1,\dots,N_E, \tag{5}$$

Finally, we suppose known the convex functions $f_j \in C^2(0,\infty)$, (the treatment cost of the discharge in the point P_j, $j=1,\dots,N_E$) and, consequently, the global cost of the depuration system in a time interval $[0,T]$, which is given by

$$J(m) = \sum_{j=1}^{N_E} \int_0^T f_j(m_j(t))\,\mathrm{d}t. \tag{6}$$

Then the problem, denoted by $(\mathscr{P})$, of the optimal management of the depuration systems consists of finding the values of BOD $m_j(t)$, $j=1,\dots,N_E$, throughout the time interval in such a way that, verifying the state system (1), satisfy the constraints (3)–(5) and minimize the cost function (6).

3. The discretized problem

The first step in the numerical resolution of the problem is solving the state system (1). In order to do it, we choose a number $N\in\mathbb{N}$ and define

$$\Delta t = \frac{T}{N} > 0$$

and $t_n = n\Delta t$, $\forall n=0,\dots,N$. Moreover, we take a triangulation τ_h of Ω with vertices x_j, $j=1,\dots,N_V$, and consider V_h the following finite element space:

$$V_h = \{v_h \in C^0(\overline{\Omega}):\ v_{h|K}\in P_1,\ \forall K\in\tau_h\}. \tag{7}$$

Then, we carry out a time discretization of the partial differential equations system (1) and we consider the variational formulation of the semi-discretized problem. Thus, using finite elements techniques, the resultant problem is equivalent to solving the following linear system:

$$\begin{aligned} M_{1h}\rho_{1h}^{n+1} &= b_{1h}^n, \quad \forall n=0,\dots,N-1,\\ M_{2h}\rho_{2h}^{n+1} &= b_{2h}^n, \quad \forall n=0,\dots,N-1, \end{aligned} \tag{8}$$

for ρ_{1h}^0 and ρ_{2h}^0 given, and where ρ_{1h}^n and ρ_{2h}^n are numerical approximation of ρ_1 and ρ_2 at the time t_n and at every vertex of the triangulation, and M_{1h}, M_{2h}, b_{1h}^n, b_{2h}^n are the matrices and second member vectors for the finite elements discretization (see [11] for further details).

The discretized cost $\hat{J}$ and the discretized constraints g are given by

$$\begin{aligned} &\hat{J} : \mathbb{R}^{N\times N_{\mathrm{E}}} \to \mathbb{R} \\ &m \to \hat{J}(m) = \Delta t \sum_{j=1}^{N_{\mathrm{E}}} \sum_{n=0}^{N-1} Q_{jn} f_j(m_{jn}), \\ &g : \mathbb{R}^{N\times N_{\mathrm{E}}} \to \mathbb{R}^{N\times N_{\mathrm{VZ}}} \times \mathbb{R}^{N\times N_{\mathrm{VZ}}} \times \mathbb{R}^{N\times N_{\mathrm{E}}} \\ &m \to g(m) = (\underbrace{\tilde{\rho}_{1h} - \sigma,\ \zeta - \tilde{\rho}_{2h}}_{=g_1(m)}, \underbrace{\underline{m} - m}_{=g_2(m)})^t, \end{aligned} \tag{9}$$

where m is the vector consisting of all of the discharges at all times, m_{jn} is the amount of BOD discharged in P_j at time t_n, Q_{jn} are the weights of the quadrature formula, N_{VZ} is the number of vertices in the protected zones and $\tilde{\rho}_{ih}$ is a vector of values of ρ_{ih} at vertices included in the protected areas for all times.

Then, the optimal control problem $(\mathscr{P})$ is approximated by the following discretized problem with convex objective function and linear constraints:

$$(\mathscr{P}_{\mathscr{F}}) \quad \begin{cases} \min\limits_{m\in\mathbb{R}^{N\times N_{\mathrm{E}}}} \hat{J}(m), \\ \text{such that } g(m)\leqslant 0. \end{cases} \tag{10}$$

4. Numerical resolution

In order to check the results of the numerical resolution of the problem $(\mathscr{P}_{\mathscr{F}})$ we have used two different methods: an admissible points method and a successive quadratic programming algorithm.

4.1. An admissible points algorithm

Firstly we have solved the problem $(\mathscr{P}_{\mathscr{F}})$ by means of an admissible points method which is based on a globally convergent algorithm introduced by Herskovits [5] and Panier et al. [9] for nonlinear constraint problems.

If we denote the dimension of the control by p, the number of the constraints on the state by q and the vector of the dual variables by $(\lambda,\theta)\in\mathbb{R}^{p\times q}$, then we can write the first order Karush–Kuhn–Tucker optimality conditions for our problem as follows:

$$\nabla\hat{J}(m) + \nabla g_1\lambda - I\theta = 0, \qquad G_1(m)\lambda = 0, \qquad G_2(m)\theta = 0, \tag{11}$$

$$\lambda\geqslant 0, \qquad \theta\geqslant 0, \qquad g_1(m)\leqslant 0, \qquad g_2(m)\leqslant 0, \tag{12}$$

where $G_1(m)$ and $G_2(m)$ are diagonal matrices of order q and p, respectively, and with diagonal elements being the values of the corresponding functions $g_i(m)$.

The basic idea of the admissible points algorithm consists of solving the system of equations (11) in (m,λ,θ) by using a fixed point method, in such a way that the conditions (12) hold at each iteration.

If we denote $H(m,\lambda,\theta) = \nabla^2\hat{J}(m) + \sum_{i=1}^{q} \lambda_i\nabla^2 g_{1i}(m) + \sum_{j=1}^{p} \theta_j\nabla^2 g_{2j}(m)$ the Hessian of the Lagrangian and Λ^k, Θ^k two diagonal matrices of order q and p, respectively, with $(\Lambda^k)_{ii} = (\lambda^k)_i$ and

Table 1
Sketch of the admissible points algorithm

Step 0	(1) Compute $g_1(0)$, ∇g_1 (2) Choose $(m^0,\lambda^0,\theta^0)^t$ such that $g(m^0)\leqslant 0$, $\lambda^0\geqslant 0$, $\theta^0\geqslant 0$
Step 1	Compute the descent direction d^k by solving the linear system: $\begin{pmatrix} H(m^k,\lambda^k,\theta^k) & \nabla g_1 & -I \\ \Lambda^k(\nabla g_1)^t & G_1^k & 0 \\ -\Theta^k & 0 & G_2^k \end{pmatrix}\begin{pmatrix} d^k \\ \lambda_0^{k+1} \\ \theta_0^{k+1}\end{pmatrix}=\begin{pmatrix}-\nabla\hat{J}(m^k) \\ 0 \\ 0\end{pmatrix}$ (13)
Step 2	Compute the step length t^k by employing a line search technique and define $m^{k+1}=m^k+t^kd^k$
Step 3	Update the dual variable: define $(\lambda^{k+1},\theta^{k+1})$ from $(\lambda_0^{k+1},\theta_0^{k+1})$
Step 4	Convergence Test: (1) If OK $\rightarrow$ stop algorithm and accept m^{k+1} as solution of the problem $(\mathscr{P}_{\mathscr{F}})$ (2) If not OK $\rightarrow$ return to Step 1

$(\Theta^k)_{jj}=(\theta^k)_j$, then the general sketch of the algorithm, applied to our problem, is given in Table 1 (cf. [8] for further details).

We can analyse now the main aspects of the algorithm:

Step 0: A simple way in order to compute the rows of ∇g_1 is linearizing with respect to m the system (8) and solving it for the vectors of the canonical basis (cf. [8]).

Step 1: We must note that:

(1) Denoting $H^k=H(m^k,\lambda^k,\theta^k)$, since constraints are linear, we have that $H^k=\nabla^2\hat{J}(m^k)$. Moreover, the particular form of the functional $\hat{J}$ causes H^k to be diagonal and easy to compute.

(2) The fact that $f_j(m)$, $j=1,\ldots,N_{\rm E}$, are strictly convex in the minimization interval guarantees that H^k is positive definite and, consequently, if (λ^k,θ^k) are such that:
   (a) $(\lambda^k)_i>0$, if $(g_1(m^k))_i=0$,
   (b) $(\theta^k)_j>0$, if $(g_2(m^k))_j=0$,
   (strict complementarity slackness) then the matrix of system (13) is nonsingular (cf. [9]).

Thus, we have obtained a nonsingular linear system of order $2p+q$, where the only nondiagonal blocks are $\nabla g_1\in\mathscr{M}_{p\times q}$ and $\Lambda^k(\nabla g_1)^t\in\mathscr{M}_{q\times p}$. If the values of p (dimension of the control variable) and q (number of linear constraints that are not bound constraints) are not very large, system (13) can be simply solved, for instance, by a preconditionated biconjugate gradient method. However, when p and q grow, the necessity of preconditioning at each iteration makes this method very slow.

In this case, a possible alternative is to solve the system by computing by blocks. So, system (13) can be written as

$$H^kd^k+\nabla g_1\lambda_0^{k+1}-I\theta_0^{k+1}=-\nabla\hat{J}(m^k), \quad (14)$$

$$\Lambda^k(\nabla g_1)^t d^k + G_1^k \lambda_0^{k+1} = 0, \tag{15}$$

$$-\,\Theta^k d^k + G_2^k \theta_0^{k+1} = 0. \tag{16}$$

Taking into account that in our problem $q > p$, a first strategy consists of computing λ_0^{k+1} and θ_0^{k+1} from (15) and (16), respectively, and substituting them into (14), which leads us to the following system in d^k:

$$[H^k - \nabla g_1 (G_1^k)^{-1} \Lambda^k (\nabla g_1)^t - (G_2^k)^{-1} \Theta^k] d^k = -\nabla \hat{J}(m^k). \tag{17}$$

This system is only of order p and, whenever G_1^k and G_2^k are nonsingular, the matrix of the system is symmetric and positive definite (see [6]). Thus, it can be solved, for instance, by Choleski method.

Nevertheless, this strategy cannot be developed when G_1^k or G_2^k are singular, and it is even problematical if any of the diagonal elements of these matrices is close to zero, because in this case system (17) is strongly ill-conditioned. An alternative strategy in order to allow this problem is to determine previously the constraints close to saturation (*active constraints*) and compute in (15) and (16) only those variables $(\lambda_0^{k+1})_i$, $(\theta_0^{k+1})_j$ associated to inactive constraints. In this way, (17) is only completely solved at those iterations where no constraint is fulfilled. In the case of active constraints, instead of (17), we have the following system:

$$\begin{pmatrix} B^k & \widetilde{\nabla g_1} & -\tilde{I} \\ \tilde{\Lambda}^k (\widetilde{\nabla g_1})^t & \widetilde{G_1^k} & 0 \\ -\tilde{\Theta}^k & 0 & \widetilde{G_2^k} \end{pmatrix} \begin{pmatrix} d^k \\ \tilde{\lambda}_0^{k+1} \\ \tilde{\theta}_0^{k+1} \end{pmatrix} = \begin{pmatrix} -\nabla \hat{J}(m^k) \\ 0 \\ 0 \end{pmatrix}, \tag{18}$$

where the elements with *tilde* are obtained taking the rows and columns associated to active constraints in the corresponding elements, and $B^k \in \mathscr{M}_{p\times p}$ is a matrix similar to the one of system (17) where divisions by values close to zero have been eliminated.

This system is of lower order and, although nonsymmetric, is better conditioned than (17). Thus, for its resolution a QR factorization can be used.

We must also remark that matrix B^k is full, which implies a great computational effort. We can introduce a possible variant in order to obtain B^k diagonal, assuming (taking into account condition (11)) that the coordinates of the dual variable $(\lambda^k, \theta^k)^t$ not associated to active constraints are null. This assumption, that must be taken in mind in Step 3, makes B^k diagonal and, consequently, the resolution of system (18) becomes quicker (now, a preconditionated biconjugate gradient method can be used). In this case, a correction of the descent direction must be introduced in order to assure convergence.

Step 2: Since the constraints of our problem are linear, we have chosen the following modification of Armijo's rule (cf. for instance [7]):

Let $\eta, v \in (0,1)$. For $m^k, d^k \in \mathbb{R}^p$ given:

(1) We compute $t_{\max}^k$, the largest step such that $m^k + t_{\max}^k d^k$ verifies all the contraints (simple because of the linearity of the constraints).

(2) We choose $l \geqslant 0$ the first natural number such that

$$\hat{J}(m^k + v^l t^k_{\max} d^k) \leqslant \hat{J}(m^k) + \eta v^l t^k_{\max} (\nabla \hat{J}(m^k))^t d^k. \tag{19}$$

(3) We take $t^k = v^l t^k_{\max}$ and, finally, we define $m^{k+1} = m^k + t^k d^k$.

Step 3: In order to update the values of the dual variable $(\lambda_0^{k+1}, \theta_0^{k+1})^t$ we have used two different variants:

Variant 1: We take ξ_1, ξ_2, μ_1, μ_2, λ^I, θ^I positive and:

(1) $\forall i = 1, \ldots, q$, $\forall j = 1, \ldots, p$, we define

$$(\lambda^{k+1})_i = \sup\{(\lambda_0^{k+1})_i,\ \xi_1 \|d^k\|^2\}, \tag{20}$$

$$(\theta^{k+1})_j = \sup\{(\theta_0^{k+1})_j,\ \xi_2 \|d^k\|^2\}, \tag{21}$$

(2) if $(g_1(m^{k+1}))_i \geqslant -\mu_1$ and $(\lambda^{k+1})_i < \lambda^I$, we redefine $(\lambda^{k+1})_i = \lambda^I$

(3) if $(g_2(m^{k+1}))_j \geqslant -\mu_2$ and $(\theta^{k+1})_j < \theta^I$, we redefine $(\theta^{k+1})_j = \theta^I$

Variant 2: If we consider that the coordinates of the dual variable $(\lambda^k, \theta^k)^t$ associated to inactive constraints are zero, then a modification of previous algorithm is necessary. Thus, the update of the dual variable must be made in the following way:

(1) we start with $(m^0, \lambda^0, \theta^0)^t$ such that $g(m^0) < 0$, $\lambda^0 = 0$, $\theta^0 = 0$.

(2) let $\varepsilon > 0$ be small. For $k = 0, 1, 2, \ldots$, we define

$$\begin{aligned} &(\lambda^{k+1})_i = \sup\{(\lambda_0^{k+1})_i,\ \lambda^I\} && \text{if } -\varepsilon \leqslant (g_1(m^k))_i \leqslant 0, \\ &(\lambda^{k+1})_i = 0 && \text{otherwise,} \end{aligned} \tag{22}$$

$$\begin{aligned} &(\theta^{k+1})_j = \sup\{(\theta_0^{k+1})_j,\ \theta^I\} && \text{if } -\varepsilon \leqslant (g_2(m^k))_j \leqslant 0, \\ &(\theta^{k+1})_j = 0 && \text{otherwise,} \end{aligned} \tag{23}$$

4.2. A successive quadratic programming algorithm

In order to check the numerical results, we have also solved the problem $(\mathscr{P}_{\mathscr{F}})$ by means of the successive quadratic programming algorithm OPTR05, developed by Pola [10]. The sketch of the algorithm, applied to our problem, is as follows: we consider the matrix C and the vector b defined by

$$\forall j = 1, \ldots, q: \quad C_j = \nabla (g_1)_j,\ b_j = -(g_1(0))_j,$$

$$\forall j = q+1, \ldots, q+p: \quad C_j = (0, \ldots, \underbrace{-1}_{\text{location } j}, \ldots, 0)^t,\ b_j = -(\underline{m})_j, \tag{24}$$

then we rewrite problem $(\mathscr{P}_{\mathscr{F}})$ in the following equivalent way:

$$(\mathscr{P}'_{\mathscr{F}}) \begin{cases} \min\limits_{m \in \mathbb{R}^p} \hat{J}(m) \\ \text{such that } (C_j)^t m \leqslant b_j,\ \forall j = 1, \ldots, p+q. \end{cases} \tag{25}$$

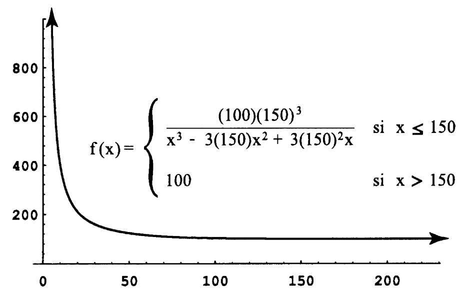

Fig. 3. Cost function.

Table 2
Parameters for the problem on Vigo's *ría*

Saint-Venant parameters	Empiric coefficients	Adimensional constants
Tidal cycle: $T=12.4$ h	$\beta_1=\beta_2=2000$ m^2/s	$N=120$
Tidal run: 2.8 m	$\kappa_1=1.15\times10^{-5}$ s^{-1}	$\xi_1=10^{-8}$
Water density: 1000 kg/m^3	$\kappa_2=9\times10^{-12}$ s^{-1}	$\xi_2=10^{-8}$
Air density: 1.28 kg/m^3	$d_s=8.98\times10^{-3}$ kg/m^3	$\mu_1=10^{-5}$
North latitude: 0.73266 rad	$\rho_{10}=0$ kg/m^3	$\mu_2=10^{-5}$
Wind direction: 3.92699 rad	$\rho_{20}=8.082\times10^{-3}$ kg/m^3	$\lambda^I=1$
Wind velocity: 10 km/h	$\sigma_1=3.48398\times10^{-4}$ kg/m^3	$\theta^I=1$
Earth angular velocity:	$\sigma_2=5\times10^{-4}$ kg/m^3	
7.92×10^{-5} rad/s	$\zeta_1=8.05255\times10^{-3}$ kg/m^3	
	$\zeta_2=8.03218\times10^{-3}$ kg/m^3	
	$\underline{m}=0$ kg	

The basic idea of this algorithm is solving $(\mathscr{P}'_{\mathscr{F}})$ by an iterative method, in such a way that a quadratic problem with linear constraints be solved at each iteration. Concretely, at the iteration $k+1$, for a given admissible point m^k, we denote $p^k=\nabla\hat{J}(m^k)$ and $B^k=\nabla^2\hat{J}(m^k)$, and we consider the following second-order approximation of $\hat{J}$ in the neighborhood of m^k:

$$\hat{J}(m)\simeq\hat{J}(m^k)+(p^k)^t(m-m^k)+\tfrac{1}{2}(m-m^k)^tB^k(m-m^k), \tag{26}$$

defining $d=m-m^k$ we can rewrite the previous expression as follows:

$$\hat{J}(m)\simeq\underbrace{\tfrac{1}{2}d^tB^kd+(p^k)^td}_{q^k(d)}+\hat{J}(m^k). \tag{27}$$

Descent direction d^k is determined as the solution of the quadratic problem:

$$(\mathscr{P}_{\mathscr{Q}})^k\begin{cases}\min\limits_{d\in\mathbb{R}^p} q^k(d),\\ \text{such that } (C_j)^td\leqslant b_j-C_j^tm^k,\ \forall j=1,\dots,p+q\end{cases} \tag{28}$$

and step t^k is computed by using line search techniques. Thus, we finally define $m^{k+1}=m^k+t^kd^k$.

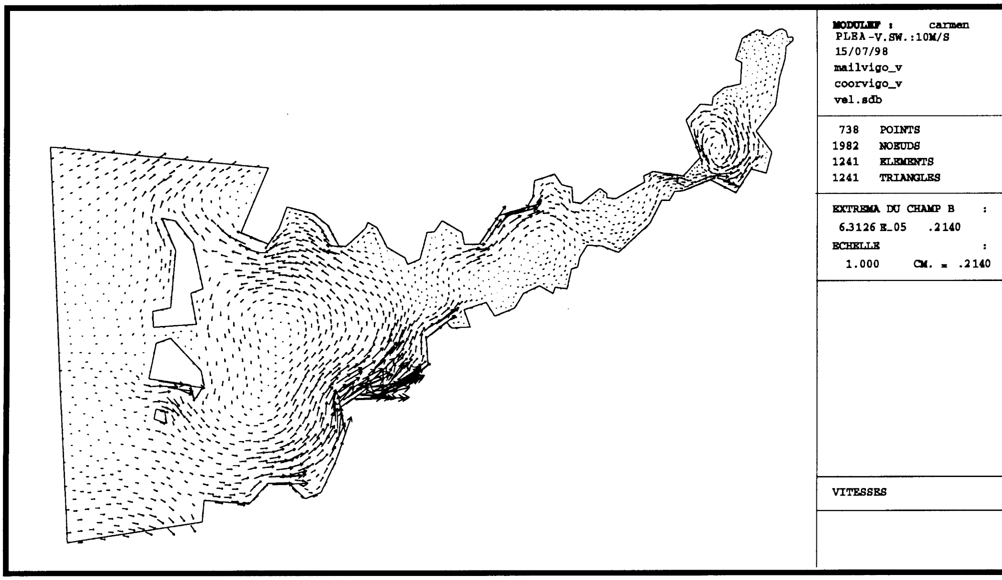

Fig. 4. Velocity field at high tide.

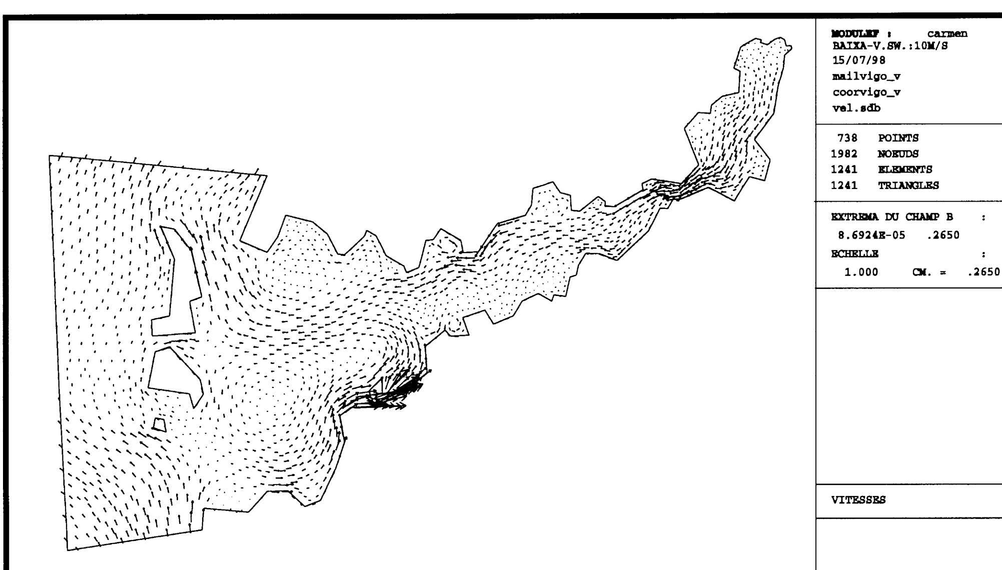

Fig. 5. Velocity field at low tide.

As can be seen, at each iteration, a quadratic problem has to be solved, which has only one solution because B^k is positive definite. In order to compute this solution, an active constraints algorithm has been used. This algorithm (cf. [4]) is very suitable for this case, because the number of saturated constraints in our problem is small.

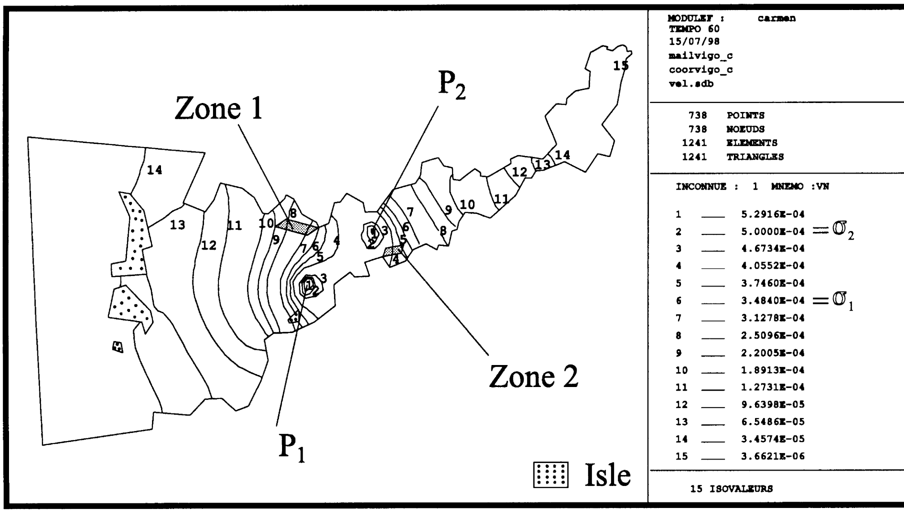

Fig. 6. BOD concentration at high tide.

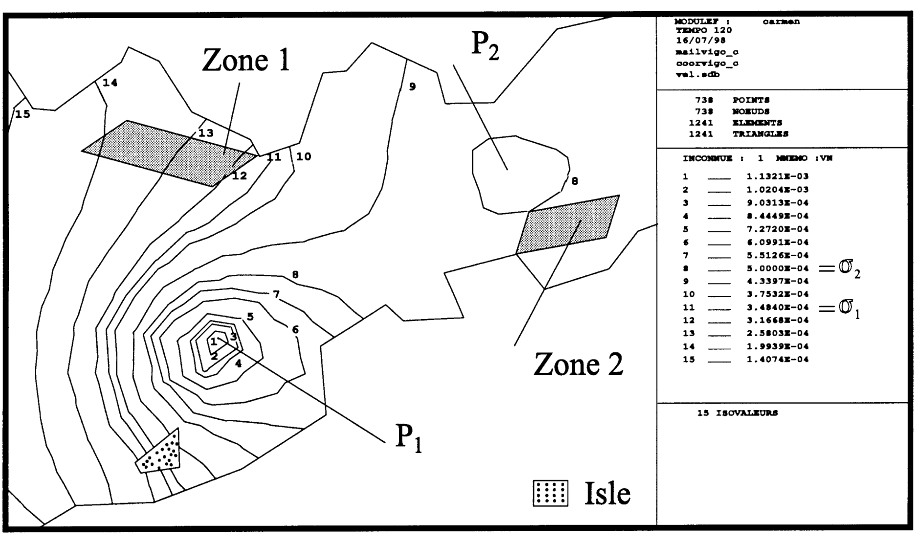

Fig. 7. BOD concentration at low tide (detail).

5. Numerical results

We have solved the problem $(\mathscr{P}_{\mathscr{F}})$ under realistic hypotheses: we have taken a two-dimensional mesh of Vigo's *ría* (Spain) as domain Ω, where we have considered two zones to protect and two points of discharge (see Figs. 6 and 7). We have also assumed that it is necessary to guarantee lower levels of pollution in zone 1 than in zone 2. (The values of all the parameters can be seen in Table 2).

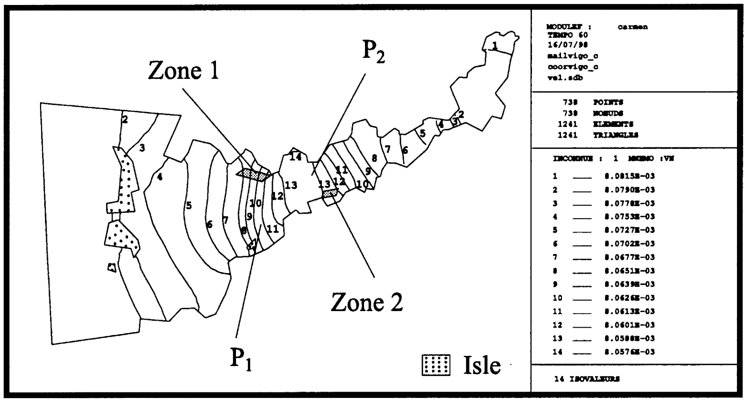

Fig. 8. DO concentration at high tide.

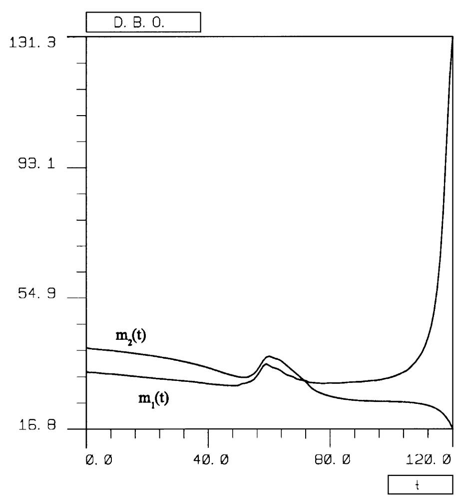

Fig. 9. Optimal discharges during a tidal cycle.

The cost function is given in Fig. 3: we assume pollutant concentration of the sewage arriving to the sewage farm is 150 kg/m^3, then the depuration cost above this value is constant. The velocity and the height of the water have been obtained solving the Saint–Venant equations on this domain (Figs. 4 and 5 show the velocity field at two significant instants). The numerical resolution of the Saint–Venant equations has been carried out in [3].

Figs. 6 and 7 show the BOD concentration at high tide and at low tide, respectively. The constraints are satisfied everywhere in the protected areas: at high tide, they saturate at one of the vertices in zone 1, but at low tide, after a tidal cycle, the saturation takes place at one vertex in zone 2. The DO concentration at high tide is also shown in Fig. 8.

The values of the optimal discharges, which produce this situation, can be seen in the Fig. 9. The discharge rate during rising tide is greater at point P_2 than at point P_1. However, during ebb tide (after 60 time steps) the flow rate decreases at P_2 and increases at P_1. This is an obvious consequence of the outfalls position: in fact, during rising tide, P_2 is a better location than P_1, but during ebb tide, P_1 is the best of them.

We must remark that, in all the tests we have developed, applying both methods above exposed, the results have been almost the same. Moreover, the running times are similar, if in the admissible points algorithm the update of the dual variable is made according to the size of the problem: the first variant for small values of p and q, and the second for larger ones.

References

[1] A. Bermúdez, Mathematical techniques for some environmental problems related to water pollution control, in: J.I. Díaz, J.L. Lions (Eds.), Mathematics, Climate and Environment, Masson, París. 1993.

[2] A. Bermúdez, A. Martínez, C. Rodríguez, Un probleme de controle ponctuel lie a l'emplacement optimal d'emissaires d'evacuation sous-marine, C. R. Acad. Sci. Paris, Serie I 313 (1991) 515.

[3] A. Bermúdez, C. Rodríguez, M.A. Vilar, Solving shallow water equations by a mixed implicit finite element method, IMA J. Numer. Anal. 11 (1991) 79.

[4] E. Casas, C. Pola, A sequential generalized quadratic programming algorithm using exact L_1 penalty functions, Optim. Methods Software 2 (1993) 145.

[5] J. Herskovits, A two stage feasible directions algorithm for nonlinear constrained optimization, Math. Programm. 36 (1986) 19.

[6] J. Herskovits, A feasible directions interior point technique for nonlinear optimization, J. Optim. Theory Appl. 99 (1998) 121.

[7] J.B. Hiriart-Urruty, C. Lemarechal, Convex Analysis and Minimization Algorithms, Springer, Berlin, 1993.

[8] A. Martínez, C. Rodríguez, M.E. Vázquez-Méndez, Theoretical and numerical analysis of an optimal control problem related to wastewater treatment, Preprint, Dept. Matemática Aplicada, Univ. Santiago de Compostela, Spain, 1998.

[9] E.R. Panier, A.L. Tits, J. Herskovits, A QP-free, globally convergent, locally superlinearly convergent algorithm for inequality constrained optimization, SIAM J. Control Optim. 26 (1988) 788.

[10] C. Pola, Algoritmos Numéricos para la resolución de problemas de optimización con restricciones, Ph.D. Thesis, Univ. Cantabria, Spain, 1992.

[11] M.E. Vázquez-Méndez, Contribución a la resolución numérica de modelos para el estudio de la contaminación de aguas, Master Thesis, Dept. Matemática Aplicada, Univ. Santiago de Compostela, Spain, 1992.