Numerical optimization for the purification of polluted shallow waters

L.J. Alvarez-Vázquez\textsuperscript{a}, A. Martínez\textsuperscript{a}, R. Muñoz-Sola\textsuperscript{b}, C. Rodríguez\textsuperscript{b}, M.E. Vázquez-Méndez\textsuperscript{c,}\textsuperscript{*}

\textsuperscript{a}Departamento de Matemática Aplicada II, ETSI Telecomunicación, Universidad de Vigo, 36200 Vigo, Spain
\textsuperscript{b}Departamento de Matemática Aplicada, Facultad de Matemáticas, Universidad de Santiago de Compostela, 15782 Santiago, Spain
\textsuperscript{c}Departamento de Matemática Aplicada, Escola Politécnica Superior, Universidad de Santiago de Compostela, 27002 Lugo, Spain

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Abstract

The optimal control theory allows us to design a wastewater treatment system in order to control marine pollution in any open area of shallow waters, as was shown in previous works of the authors. However, there exist many closed areas (for instance, enclosed bays) which present a serious quality problem caused by domestic/industrial contaminants, due to the insufficient seawater exchange. In these areas it is necessary to consider a new technique in order to purify polluted waters: promoting seawater exchange by the injection of clear water from the outer sea.

The aim of this paper is to determine the minimal quantity of injected water in order to purify the protected areas up to a fixed threshold. We present the mathematical formulation of the continuous and discretized control problems, and propose an algorithm for the numerical resolution. Finally, we present numerical results obtained in the study of a real-world problem.

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\textsuperscript{*}Corresponding author. Tel.: +34 982 252 231; fax: +34 982 285 926.
E-mail addresses: lino@dma.uvigo.es (L.J. Alvarez-Vázquez), aurea@dma.uvigo.es (A. Martínez), rafa@zmat.usc.es (R. Muñoz-Sola), carmen@zmat.usc.es (C. Rodríguez), ernesto@lugo.usc.es (M.E. Vázquez-Méndez).

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1. Introduction: the ecological problem

Contaminants are classified into four main types regarding their sources: natural, domestic, industrial and agricultural contaminants. All of these can arrive into the sea by river discharges, atmospheric transport, wastewater discharges or industrial waste disposal, and, generally, cause the pollution of the marine environment. The impact of contaminants into environment is highly dependent on both their quantity/concentration and the morphology of water region into which they are discharged. Protection of the marine environment is developed by means of water quality and emission standards, limiting the maximum concentration and the quantity of contaminants to be discharged into the sea (we can recall, for instance, the directives of the Council of European Communities concerning the discharge of dangerous substances, the quality of bathing water or the quality of shellfish waters). Coastal pollution is generally controlled by treating contaminants at origin or at sewage farms by chemical/biological methods in order to reduce their concentration. In practice, several control parameters can be used (dissolved oxygen, temperature, biochemical oxygen demand, pH, heavy metals concentration, radioactivity...), all of them indicating the water quality. In order to avoid sanitary problems, it is necessary to guarantee a minimum or maximum level of the parameter in each area to be protected: fisheries, bathing zones, marine recreation areas and so on.

Two related optimal control problems have been recently studied by the authors, both from the theoretical and numerical point of view. The main aims were to obtain the optimal level of the discharges and the optimal location of wastewater outfalls in order to minimize the global purification cost and to guarantee the water quality standards (see Martínez et al. ([8,9]) and Alvarez-Vázquez et al. ([3,4])). The optimal control theory allows us to design a wastewater treatment system in order to control marine pollution in any open area of shallow waters. However, there exist many closed areas (for instance, enclosed bays) which present an important quality problem caused by domestic and/or industrial contaminants, due to the insufficient seawater exchange. In these areas where the ability of natural purification is very weak, it is necessary to consider a new technique in order to purify polluted waters: the most common strategy consists of promoting seawater exchange by the injection of clear water from the outer sea. This strategy presents a high efficiency to purify polluted closed areas in a short period of time. In this process of water conveyance the main problem consists, once the injection point is selected by geophysical reasons, of finding the minimum quantity of water which is needed to be injected into the closed area in order to purify it up to a fixed threshold. The goal of this paper is to determine this minimal quantity of injected water in order to ensure that the contaminant concentration in the protected areas is lower than fixed thresholds. Mathematically, this is a parabolic optimal control problem with constraints on the control variables.

In Section 2 we present the mathematical formulation of the continuous problem. Next section is devoted to the derivation of optimality conditions in order to characterize the optimal solutions. In Section 4 we deal with the discretization of the control problem by means of a characteristics-mixed finite elements method, obtaining the discretized adjoint system and the gradient of the cost function. Finally, last section is devoted to the numerical resolution of a realistic problem, where the optimization algorithm is introduced and computational results are provided.
2. Mathematical formulation of the problem

We consider a domain $\Omega \subset \mathbb{R}^2$ of shallow waters (for instance a ría, an estuary or a lake) where we suppose domestic wastewater discharges through $L$ submarine outfalls located at points $b_j \in \Omega$, $j = 1, \ldots, L$. As usual, we take faecal coliphorm bacteria as indicator of the water quality (in domestic wastewater, its concentration is much greater than for other microorganisms) and we assume the existence of a highly polluted area $A = \bigcup_{k=1}^R A_k \subset \Omega$, for example an enclosed bay with poor seawater exchange, where we need to guarantee the water quality with levels of coliphorm concentration lower than maximum previously fixed value $c$.

In order to purify the region $A$ we inject clear water through a portion $\Gamma^-$ of the boundary of $\Omega$. We consider the remainder of the boundary of $\Omega$ divided into two parts: $\Gamma^0$ (corresponding to the coast) and $\Gamma^+$ (corresponding to open sea) in such a way that $\partial \Omega = \Gamma^- \cup \Gamma^0 \cup \Gamma^+$. We denote by $H(x, t)$, $\vec{u}(x, t)$ and $\rho(x, t)$, respectively, the height of water, the depth-averaged horizontal velocity of water and the depth-averaged coliphorm concentration at any point $x \in \Omega$ and any time $t \in (0, T)$. The evolution of $H$, $\vec{u}$ and $\rho$ along $\Omega \times (0, T)$ is obtained as the solution of the boundary value problem coupling the shallow water equations with the convection–diffusion–reaction equation for the coliphorm concentration:

$$\begin{align*}
\frac{\partial H}{\partial t} + \vec{\nabla}.(H \vec{u}) &= 0 \quad \text{in } \Omega \times (0, T), \\
\frac{\partial \vec{u}}{\partial t} + (\vec{u}.\vec{\nabla}) \vec{u} - v \vec{\nabla}(\vec{\nabla}.\vec{u}) + g \vec{\nabla}H &= \vec{F} \quad \text{in } \Omega \times (0, T), \\
\frac{\partial \rho}{\partial t} + \vec{u}.\vec{\nabla} \rho + k \rho - \beta \Delta \rho &= \frac{1}{H} \sum_{j=1}^L m_j \delta(x - b_j) \quad \text{in } \Omega \times (0, T), \\
H &= \eta \quad \text{on } \Gamma^- \times (0, T), \\
H &= \phi \quad \text{on } \Gamma^+ \times (0, T), \\
H(0) &= H_0 \quad \text{in } \Omega, \\
\vec{u}.\vec{n} &= q \quad \text{on } \Gamma^- \times (0, T), \\
\vec{u}.\vec{n} &= 0 \quad \text{on } \Gamma^0 \times (0, T), \\
\vec{\nabla}.\vec{u} &= 0 \quad \text{on } \Gamma^+ \times (0, T), \\
\vec{u}(0) &= \vec{u}_0 \quad \text{in } \Omega, \\
\rho &= 0 \quad \text{on } \Gamma^- \times (0, T), \\
\frac{\partial \rho}{\partial n} &= 0 \quad \text{on } (\Gamma^+ \cup \Gamma^0) \times (0, T), \\
\rho(0) &= \rho_0 \quad \text{in } \Omega, 
\end{align*}$$

(1)
where \( \delta(x - b_j) \), \( j = 1, \ldots, L \), denotes the Dirac measure at point \( b_j \), \( m_j(t) \) is the mass flow rate of coliphorm discharged in \( b_j \), \( \bar{n} \) denotes the unit outer normal vector to boundary \( \partial \Omega \), and the second member \( \vec{F} \) collects all the effects of atmospheric pressure, wind stress, bottom friction and so on. We also assume all the physical parameters experimentally known: \( \nu \) the coefficient of kinetic eddy viscosity, \( g \) the gravity acceleration, \( \beta \) the horizontal viscosity coefficient and \( k \) a kinetic parameter related to temperature. The boundary conditions on the injection boundary \( \Gamma^- \) correspond to the height of injected water (assumed to be fixed), the velocity of clear water \( q \) (which will be the control of our problem) and the coliphorm concentration (assumed to be zero, since we are injecting clear water). The other boundary conditions on the coast \( \Gamma^0 \) and the open sea \( \Gamma^+ \), as much as the initial conditions, are classical (cf. [12] or [1]).

Since we need to inject water through \( \Gamma^- \) we are led to consider only the admissible velocities in the set:

\[
U_{ad} = \{ l \in L^2(0, T; L^2(\Gamma^-)) : 0 \geq l \}. \tag{2}
\]

We formulate the control problem considering as the cost functional the total amount of clear water injected through \( \Gamma^- \) together with a measure in the region \( A \) of the coliphorm concentration which remains higher than the fixed threshold \( c \). Thus, we define the cost function:

\[
J(q) = \frac{m}{2} \int_0^T \int_{\Gamma^-} \eta^2 q^2 + \frac{n}{2} \int_0^T \int_A (\rho - c)^2 + \vec{n} \cdot \vec{v}^2, \tag{3}
\]

where \( m \) and \( n \) are two positive weight parameters, related to the role played by the amount of clear water and the fulfilment of the quality constraints in the objective function.

Then the problem, denoted by \( \mathcal{P} \), of the optimal water conveyance for the purification of polluted areas consists of finding the control velocity \( q \in U_{ad} \) of injected clear water in such a way that, verifying the state system (1), minimizes the cost function \( J \) given by (3). Thus, the problem can be written as

\[
\mathcal{P} \quad \min_{q \in U_{ad}} J(q). \]

3. Analysis of the optimal control problem

Existence, uniqueness and regularity for the solutions to shallow water equations is still an open problem in the general case, although several results for particular cases have been achieved (one of the first attempts to deal with the well-posedness of the shallow water equations was due to Ton [14] more than two decades ago). From a numerical point of view the contributions have been more numerous: several numerical approximations of \( H \) and \( \vec{u} \) have been obtained by finite difference, finite element or finite volume methods. For the solution of the coliphorm concentration equation starting from an achieved solution of the shallow water equations several crucial results can be seen, for instance, in [8].

All along this work we will extensively use the method of characteristics, which stems from considering the following equality:

\[
\frac{Dy}{Dt}(x, t) = \frac{\partial y}{\partial x}(x, t) + \vec{u} \cdot \vec{n},
\]
where \( \frac{Dy}{Dt} \) denotes the total derivative of \( y \) with respect to \( t \) and \( \vec{u} \), that is

\[
\frac{Dy}{Dt} (x, t) = \frac{\partial y}{\partial \tau} (X(x, t; \tau), \tau)|_{\tau=t},
\]

with \( \tau \rightarrow X(x, t; \tau) \) the characteristic line, providing the position at time \( \tau \) of the particle that occupied the position \( x \) at time \( t \). So, the characteristic line is the unique solution of the following ordinary differential equation:

\[
\frac{dX}{d\tau} (x, t; \tau) = \vec{u}(X(x, t; \tau), \tau),
\]

\( X(x, t; t) = x. \) (4)

Thus, the state system (1) can be written in the following form:

\[
\begin{align*}
\frac{DH}{Dt} + H \vec{\nabla}.\vec{u} &= 0 \quad \text{in } \Omega \times (0, T), \\
\frac{D\vec{u}}{Dt} - v \vec{\nabla}(\vec{\nabla}.\vec{u}) + g \vec{\nabla}H &= \vec{F} \quad \text{in } \Omega \times (0, T), \\
\frac{D\rho}{Dt} + k \rho - \beta \Delta \rho &= \frac{G}{H} \quad \text{in } \Omega \times (0, T), \\
H &= \eta \quad \text{on } \Gamma^- \times (0, T), \\
H &= \phi \quad \text{on } \Gamma^+ \times (0, T), \\
H(0) &= H_0 \quad \text{in } \Omega, \\
\vec{u}.\vec{n} &= q \quad \text{on } \Gamma^- \times (0, T), \\
\vec{u}.\vec{n} &= 0 \quad \text{on } \Gamma^0 \times (0, T), \\
\vec{\nabla}.\vec{u} &= 0 \quad \text{on } \Gamma^+ \times (0, T), \\
\vec{u}(0) &= \vec{u}_0 \quad \text{in } \Omega, \\
\rho &= 0 \quad \text{on } \Gamma^- \times (0, T), \\
\frac{\partial \rho}{\partial n} &= 0 \quad \text{on } (\Gamma^+ \cup \Gamma^0) \times (0, T), \\
\rho(0) &= \rho_0 \quad \text{in } \Omega,
\end{align*}
\] (5)
where, for the sake of simplicity, we denote by \( G(x, t) \) an \( L^2 \)-approximation to the measure \( \sum_{j=1}^{L} m_j(t) \delta(x - b_j) \) (cf., for instance, [7]).

The existence of solution for the optimal control problem \((\mathcal{P})\) will not be addressed here. However, the problem will be nonconvex because of the nonlinearity of the state system, so uniqueness of solution is not expected.

We will center our attention in obtaining a formal first-order optimality condition satisfied by the solutions of problem \((\mathcal{P})\). In order to express this necessary optimality condition in a simpler way we introduce the functions \((p, \vec{w}, s)\) solutions of the adjoint system:

\[
-\frac{\partial p}{\partial t} - \vec{u} \cdot \nabla p - g \vec{v} \cdot \vec{w} + \frac{s}{H^2} G = 0 \quad \text{in } \Omega \times (0, T),
\]

\[
-\frac{\partial \vec{w}}{\partial t} - \vec{v} \cdot (\vec{u} \otimes \vec{w}) + (\vec{v} \vec{u})^T \vec{w} - v \vec{v} \cdot (\vec{v} \cdot \vec{w}) - H \vec{v} p + s \vec{v} \rho = 0 \quad \text{in } \Omega \times (0, T),
\]

\[
-\frac{\partial s}{\partial t} - \vec{v} \cdot (s \vec{u}) + ks - \beta \Delta s + n_{\chi_A}(\rho - c) = 0 \quad \text{in } \Omega \times (0, T),
\]

\[
\vec{w} \cdot \vec{n} = 0 \quad \text{on } (\Gamma^- \cup \Gamma^0) \times (0, T),
\]

\[
q \vec{w} \cdot \vec{\tau} = 0 \quad \text{on } \Gamma^- \times (0, T),
\]

\[
\phi p \vec{n} + (\vec{u} \cdot \vec{n}) \vec{w} + v \vec{v} \cdot \vec{w} \vec{n} = 0 \quad \text{on } \Gamma^+ \times (0, T),
\]

\[
p(T) = 0 \quad \text{in } \Omega,
\]

\[
\vec{w}(T) = 0 \quad \text{in } \Omega,
\]

\[
s = 0 \quad \text{on } \Gamma^- \times (0, T),
\]

\[
\frac{\partial s}{\partial n} = 0 \quad \text{on } \Gamma^0 \times (0, T),
\]

\[
(\vec{u} \cdot \vec{n}) s + \beta \frac{\partial s}{\partial n} = 0 \quad \text{on } \Gamma^+ \times (0, T),
\]

\[
s(T) = 0 \quad \text{in } \Omega,
\]

where \( \vec{\tau} \) denotes the unit tangent vector to boundary \( \partial \Omega \), and \( \chi_A \) is the indicator function of the set \( A \), that is,

\[
\chi_A(x) = \begin{cases} 
1, & \text{if } x \in A, \\
0, & \text{otherwise}.
\end{cases}
\]

Thus, we can prove the following result:
Theorem 1. Let $q \in U_{ad}$ be a solution of the control problem $(P)$. Then, there exist $(H, \tilde{u}, \rho)$ solutions of the state system (1) and $(p, \tilde{w}, s)$ solutions of the adjoint system (6), such that verify the relation

$$
\int_0^T \int_{\Gamma^-} \{m\eta^2q + \eta p + v(\nabla \tilde{w})\}(l - q) \geq 0, \quad \forall l \in U_{ad}.
$$

(7)

Proof. Since $q$ is a solution of the minimization problem $(P)$, the following inequality holds:

$$
DJ(q) \cdot (l - q) \geq 0, \quad \forall l \in U_{ad}.
$$

(8)

Let $(H, \bar{u}, \rho)$ be the state corresponding to the optimal control, then we have

$$
DJ(q) \cdot (l - q) = m \int_0^T \int_{\Gamma^-} \eta^2 q(l - q) + n \int_0^T \int_A (p - c) + \tilde{\rho},
$$

where $(\bar{H}, \bar{u}, \bar{\rho}) = (D/Dq)(H, \bar{u}, \rho)(q) \cdot (l - q)$ is given by the linearized system

\begin{align*}
\frac{\partial \bar{H}}{\partial t} + \bar{\nabla} \cdot (\bar{H} \bar{u}) + \bar{\nabla} \cdot (H \bar{u}) &= 0 \quad \text{in } \Omega \times (0, T), \\
\frac{\partial \bar{u}}{\partial t} + (\bar{u} \cdot \bar{\nabla}) \bar{u} + (\bar{H} \cdot \bar{u}) \bar{u} - v\bar{\nabla} \cdot (\bar{\nabla} \bar{u}) + g\bar{\nabla} \bar{H} &= 0 \quad \text{in } \Omega \times (0, T), \\
\frac{\partial \bar{\rho}}{\partial t} + \bar{u} \cdot \bar{\nabla} \bar{\rho} + \bar{u} \cdot \bar{\nabla} \bar{\rho} + k\bar{\rho} - \beta \Delta \bar{\rho} + \frac{\bar{H}}{\bar{H}^2} G &= 0 \quad \text{in } \Omega \times (0, T), \\
\bar{H} &= 0 \quad \text{on } (\Gamma^- \cup \Gamma^+) \times (0, T), \\
\bar{H}(0) &= 0 \quad \text{in } \Omega, \\
\bar{u} \cdot \bar{n} &= l - q \quad \text{on } \Gamma^- \times (0, T), \\
\bar{u} \cdot \bar{n} &= 0 \quad \text{on } \Gamma^0 \times (0, T), \\
\bar{\nabla} \cdot \bar{u} &= 0 \quad \text{on } \Gamma^+ \times (0, T), \\
\bar{u}(0) &= 0 \quad \text{in } \Omega, \\
\bar{\rho} &= 0 \quad \text{on } \Gamma^- \times (0, T), \\
\frac{\partial \bar{\rho}}{\partial n} &= 0 \quad \text{on } (\Gamma^+ \cup \Gamma^0) \times (0, T), \\
\bar{\rho}(0) &= 0 \quad \text{in } \Omega.
\end{align*}

(9)
Thus, we have

\[ DJ(q) \cdot (l - q) = \int_0^T \int_{\Gamma^-} m\eta^2 q(l - q) + \int_0^T \int_{\Omega} n_{\mathcal{I}A}(\rho - c) + \tilde{p}, \]

\[ = \int_0^T \int_{\Gamma^-} m\eta^2 q(l - q) + \int_0^T \int_{\Omega} \left\{ \frac{\partial s}{\partial t} + \nabla \cdot (s\tilde{u}) - ks + \beta s \right\} \tilde{p}, \]

\[ = \int_0^T \int_{\Gamma^-} m\eta^2 q(l - q) + \int_0^T \int_{\Omega} \left\{ -\frac{\partial \tilde{\rho}}{\partial t} - \tilde{u} \cdot \nabla \tilde{\rho} - k\tilde{\rho} + \beta \Delta \tilde{\rho} \right\} s \]

\[ + s(T)\tilde{\rho}(T) - s(0)\tilde{\rho}(0) + \int_0^T \int_{\Gamma} \left\{ s\tilde{\rho} \tilde{n} + \beta \frac{\partial s}{\partial n} - \beta \frac{\partial \tilde{\rho}}{\partial n} \right\} s, \]

\[ = \int_0^T \int_{\Gamma^-} m\eta^2 q(l - q) + \int_0^T \int_{\Omega} \left\{ \tilde{u} \cdot \nabla \tilde{\rho} + \frac{H}{H^2} Gs \right\} s, \]

\[ = \int_0^T \int_{\Gamma^-} m\eta^2 q(l - q) + \int_0^T \int_{\Omega} \frac{H}{H^2} Gs \]

\[ + \int_0^T \int_{\Omega} \left\{ \frac{\partial \tilde{w}}{\partial t} + \nabla \cdot (\tilde{w} \otimes \tilde{w}) - (\nabla \tilde{u})^T \tilde{w} + H\tilde{v} + v \tilde{v}(\nabla \tilde{v}) \right\} \tilde{u}, \]

\[ = \int_0^T \int_{\Gamma^-} m\eta^2 q(l - q) + \int_0^T \int_{\Omega} \frac{H}{H^2} Gs \]

\[ + \int_0^T \int_{\Omega} \left\{ -\frac{\partial \tilde{u}}{\partial t} - (\tilde{u} \cdot \nabla)\tilde{u} - (\tilde{u} \cdot \nabla)\tilde{u} + v \tilde{v}(\nabla \tilde{v}) \right\} \tilde{w}, \]

\[- \int_0^T \int_{\Omega} p \tilde{v} \cdot (H\tilde{u}) + \tilde{w}(T)\tilde{u}(T) - \tilde{w}(0)\tilde{u}(0) \]

\[ + \int_0^T \int_{\Gamma} \{(\tilde{w} \cdot \tilde{u})(\tilde{u} \cdot \tilde{n}) + v(\tilde{v} \cdot \tilde{w})(\tilde{u} \cdot \tilde{n}) - v(\tilde{v} \cdot \tilde{u})(\tilde{w} \cdot \tilde{n})\} + \int_0^T \int_{\Gamma} Hp \tilde{u} \tilde{n}. \]

Taking into account that \( \{\tilde{n}, \tilde{\tau}\} \) is an orthonormal basis of \( \mathbb{R}^2 \), each vector \( \tilde{a} \in \mathbb{R}^2 \) can be written as

\[ \tilde{a} = (\tilde{a} \cdot \tilde{n})\tilde{n} + (\tilde{a} \cdot \tilde{\tau})\tilde{\tau}. \]

Then, we have that

\[ \int_0^T \int_{\Gamma} (\tilde{w} \cdot \tilde{u})(\tilde{u} \cdot \tilde{n}) = \int_0^T \int_{\Gamma^- \cup \Gamma^+} \{(\tilde{w} \cdot \tilde{u})(\tilde{u} \cdot \tilde{n}) + (\tilde{w} \cdot \tilde{\tau})(\tilde{u} \cdot \tilde{\tau})\}(\tilde{u} \cdot \tilde{n}), \]
and the other terms in a similar way. So,
\[
DJ(q) \cdot (l - q) = \int_0^T \int_{\Gamma^-} m \eta^2 q(l - q) + \int_0^T \int_{\Omega} \frac{\tilde{H}}{H^2} Gs + \int_0^T \int_{\Omega} \{g \tilde{\nabla} \tilde{H} \cdot \tilde{w} - \tilde{p} \tilde{\nabla} \cdot (\tilde{H} \tilde{u})\}
+ \int_0^T \int_{\Gamma^-} v(\tilde{\nabla} \cdot \tilde{w})(l - q) + \int_0^T \int_{\Gamma^-} \eta p(l - q),
\]
\[
= \int_0^T \int_{\Gamma^-} (m \eta^2 q + \eta p + v(\tilde{\nabla} \cdot \tilde{w}))(l - q) + \int_0^T \int_{\Omega} \frac{\tilde{H}}{H^2} Gs
+ \int_0^T \int_{\Omega} \left\{g \tilde{\nabla} \tilde{H} \cdot \tilde{w} + p \left[\frac{\partial \tilde{H}}{\partial t} + \tilde{\nabla} \cdot (\tilde{H} \tilde{u})\right]\right\},
\]
\[
= \int_0^T \int_{\Gamma^-} (m \eta^2 q + \eta p + v(\tilde{\nabla} \cdot \tilde{w}))(l - q)
+ \int_0^T \int_{\Omega} \left\{-g \tilde{\nabla} \cdot \tilde{w} - \frac{\partial \tilde{p}}{\partial t} - \tilde{u} \tilde{\nabla} \tilde{p} + \frac{s}{H^2} \tilde{G}\right\} \tilde{H}
+ p(T) \tilde{H}(T) - p(0) \tilde{H}(0) + \int_0^T \int_{\Gamma^-} \{g \tilde{H} \tilde{w} \cdot \tilde{n} + \tilde{H} \tilde{p} \tilde{u} \cdot \tilde{n}\},
\]
\[
= \int_0^T \int_{\Gamma^-} (m \eta^2 q + \eta p + v(\tilde{\nabla} \cdot \tilde{w}))(l - q).
\]

Taking this expression to (8) we obtain the desired optimality condition (7). □

4. Numerical discretization

We introduce now a discretization of the problem (P). For the time interval [0, T] we choose \( N \in \mathbb{N} \), we consider the time step \( \Delta t = T/N \) and we define \( t_n = n \Delta t, n = 0, 1, \ldots, N \). Moreover, we take \( \tau_h \) a regular finite element triangulation of \( \Omega \) (which will be assumed to be a polygonal domain of \( \mathbb{R}^2 \) from now on), where \( h \) is the discretization parameter corresponding to the maximal length of the edges in \( \tau_h \), and we define

\[
U_{\text{ad},h}^\Delta = \{l_h \in L^2(\Gamma^-) : l_h|_{\partial K \cap \Gamma^-} \in P_0, \forall K \in \tau_h; \ 0 \geq l_h\}^N.
\]

For \( n = 1, 2, \ldots, N \) we consider \( \eta^n_h \) and \( q^n_h \) suitable approximations of the boundary conditions \( \eta(., t_n) \) and \( q(., t_n) \) (obtained, for instance, by interpolation at the boundary nodes of the triangulation) and \( p^n_h \) the discretized solution of the coliphorm concentration equation at time \( t_n \) (cf. [2] for further details). Then,
we denote \( q_h^N = (q_h^1, q_h^2, \ldots, q_h^N) \) and we consider the following approximation of the cost function:

\[
J_h^N(q_h^N) = \frac{m}{2} \Delta t \sum_{n=0}^{N-1} \int_{\Gamma^-} (\eta_h^{n+1})^2 (q_h^{n+1})^2 + \frac{n}{2} \Delta t \sum_{n=0}^{N-1} \int_A (\rho_h^{n+1} - c)^2_+.
\]

The problem \((P)\) is approached by the following fully discrete control problem

\[
(P_h^N) \min_{q_h^N \in U_{ad,h}} J_h^N(q_h^N).
\]

Now, in order to obtain an approximation of the cost gradient, we introduce a discretization of the adjoint system: a characteristic scheme for time discretization and a mixed finite element method for spatial approximation. The adjoint system (6) was obtained in previous section by means of integration by parts techniques. This adjoint system can be written, by using the total derivative, in the following equivalent way:

\[
- \frac{Dp}{Dt} - g \vec{V} \cdot \vec{w} + \frac{G}{H^2} s = 0 \quad \text{in } \Omega \times (0, T),
\]

\[
- \frac{D\vec{w}}{Dt} - (\vec{V} \cdot \vec{u}) \vec{w} + (\vec{V} \vec{u})^T \vec{w} - v \vec{V} (\vec{V} \cdot \vec{w}) - H \vec{V} \rho + s \vec{V} \rho = 0 \quad \text{in } \Omega \times (0, T),
\]

\[
- \frac{Ds}{Dt} - s(\vec{V} \cdot \vec{u}) + ks - \beta s_+ + n_{IA} (\rho - c)_+ = 0 \quad \text{in } \Omega \times (0, T),
\]

\[
\vec{w} n = 0 \quad \text{on } (\Gamma^- \cup I^0) \times (0, T),
\]

\[
q \vec{w} n = 0 \quad \text{on } \Gamma^- \times (0, T),
\]

\[
\phi p n + (\vec{u} \cdot n) \vec{w} + v (\vec{V} \cdot \vec{w}) n = 0 \quad \text{on } I^+ \times (0, T),
\]

\[
p(T) = 0 \quad \text{in } \Omega,
\]

\[
\vec{w}(T) = 0 \quad \text{in } \Omega,
\]

\[
s = 0 \quad \text{on } \Gamma^- \times (0, T),
\]

\[
\frac{\partial s}{\partial n} = 0 \quad \text{on } I^0 \times (0, T),
\]

\[
(\vec{u} \cdot n) s + \beta \frac{\partial s}{\partial n} = 0 \quad \text{on } I^+ \times (0, T),
\]

\[
s(T) = 0 \quad \text{in } \Omega.
\]
For our study we will need a suitable weak formulation of the adjoint system (10). So, we consider the spaces

\[ U = H^1(\Omega), \quad V = \{ \vec{z} \in H^1(\Omega)^2 : \vec{z} \cdot \vec{n} \mid_{\Gamma^-} = 0 \}, \quad W = \{ r \in H^1(\Omega) : r \mid_{\Gamma^-} = 0 \}. \]

We will say that \((p, \vec{w}, s)\) is a weak solution to (10) if it satisfies

\[ (p, \vec{w}, s) \in L^2(0, T; U) \times L^2(0, T; V) \times L^2(0, T; W), \]

and, in the sense of distributions on \((0, T)\),

\[
- \int_{\Omega} \frac{Dp}{Dt} \vec{r} - g \int_{\Omega} \vec{\nabla} \vec{w} \cdot \vec{r} + \int_{\Omega} \frac{s}{H^2} G \vec{r} = 0, \quad \forall \vec{r} \in U, \\
- \int_{\Omega} \frac{D\vec{w}}{Dt} \vec{z} + \int_{\Omega} (\vec{u} \cdot \vec{\nabla}) \vec{w} \cdot \vec{z} + \int_{\Omega} \vec{w} \cdot (\vec{\nabla} \vec{u}) \vec{z} + \int_{\Omega} \vec{\nabla} \vec{w} \cdot \vec{\nabla} \vec{z} + \int_{\Omega} \vec{\nabla} \vec{w} \cdot \vec{\nabla} \vec{z} = 0, \quad \forall \vec{z} \in V, \\
+ \int_{\Omega} p \vec{\nabla} H \cdot \vec{z} + \int_{\Omega} p H \vec{\nabla} \vec{z} + \int_{\Omega} s \vec{\nabla} \rho \vec{z} = 0, \quad \forall \vec{z} \in V, \\
- \int_{\Omega} \frac{Dy}{Dt} s + \int_{\Omega} \vec{u} \cdot \vec{\nabla} y \cdot s + \int_{\Omega} \vec{\nabla} \vec{u} \cdot s \vec{y} + k \int_{\Omega} s y \\
+ \beta \int_{\Omega} \vec{\nabla} s \cdot \vec{\nabla} \vec{y} + n \int_{\Omega} \chi_A(\rho - c^+) y = 0, \quad \forall y \in W, \\
p(T) = 0 \quad \text{in } \Omega, \\
\vec{w}(T) = 0 \quad \text{in } \Omega, \\
s(T) = 0 \quad \text{in } \Omega. 
\]

This weak formulation will be the basis for the numerical approximations developed in this section.

In order to discretize the adjoint system (10) in time we use a first order scheme. If we denote

\[ Y^{n+1}(x) = X(x, t_n; t_{n+1}), \]

that is, the position, at time \( t_{n+1} \), of the particle that was in \( x \) at the instant \( t_n \), then the total derivative of any function \( y \) at instant \( t_n \) can be approximated by

\[
\frac{Dy}{Dt}(x, t_n) \simeq \frac{Y^{n+1}(Y^{n+1}(x)) - Y^n(x)}{\Delta t},
\]

where \( Y^n \) stands for the approximation given by \( Y^n(x) = y(x, t_n) \). Then, the adjoint system (10) can be approximated by
We take elements for approximating the pair $(x, \tilde{u})$ in the two-dimensional spaces all triangle edges. That is, we approximate the functional spaces by the nonconforming finite element constant on the edges of the triangles. In fact, they are taken as degrees of freedom. For instance, if we restrict to the reference triangle with vertices \(0,1,2\), we have continuous piecewise linear ($P_1$) functions for the height \(p^n\) and special discontinuous vector-valued functions for the velocity \(w^n\), and discontinuous piecewise linear ($P_1$) polynomials for approximating \(s^n\), where the nodes will be the midpoints of all triangle edges. That is, we approximate the functional spaces by the nonconforming finite element spaces

\[
P^N = 0, \\
\tilde{w}^N = 0, \\
s^N = 0,
\]

for \(n = N - 1, \ldots, 0:\)

\[
(p^n, \tilde{w}^n, s^n) \in U \times V \times W \text{ such that}
\]

\[
\int_{\Omega} \frac{p^n - p^{n+1} \circ Y^{n+1}}{\Delta t} r - g \int_{\Omega} \tilde{\nabla} \tilde{u}^n r + \int_{\Omega} \frac{s^n}{(H^n)^2} G^n r = 0, \quad \forall r \in U,
\]

\[
\int_{\Omega} \frac{\tilde{w}^n - \tilde{w}^{n+1} \circ Y^{n+1}}{\Delta t} \cdot z + \int_{\Omega} (\tilde{u}^n \cdot \tilde{\nabla}) \tilde{w}^n \cdot z + \int_{\Omega} \tilde{w}^n \cdot (\tilde{\nabla} \tilde{u}^n) z + \int_{\Omega} \tilde{w}^n \cdot (\tilde{\nabla} \tilde{w}^n) z + \int_{\Omega} \rho^n \tilde{w}^n \cdot z = 0, \quad \forall z \in V,
\]

\[
\int_{\Omega} \frac{s^n - s^{n+1} \circ Y^{n+1}}{\Delta t} y + \int_{\Omega} \tilde{u}^n \cdot \tilde{\nabla} s^n y + \int_{\Omega} s^n \tilde{u}^n \cdot \tilde{\nabla} y + k \int_{\Omega} s^n y + \int_{\Omega} \chi_A (\rho^n - c)_+ y = 0, \quad \forall y \in W.
\]

For spatial approximation of this semi-discretized problem we will use a mixed finite element method. We take \(\tau_h\) the regular finite element triangulation of \(\Omega\) and we will use Raviart–Thomas [13] mixed finite elements for approximating the pair \((p^n, \tilde{w}^n)\) (that is, discontinuous piecewise constant \((P_0)\) functions for the height \(p^n\) and special discontinuous vector-valued functions for the velocity \(\tilde{w}^n\)), and discontinuous piecewise linear \((P_1)\) polynomials for approximating \(s^n\), where the nodes will be the midpoints of all triangle edges. That is, we approximate the functional spaces by the nonconforming finite element spaces

\[
\begin{align*}
U_h &= \{ r_h \in L^2(\Omega) : r_h|_K \in P_0, \quad \forall K \in \tau_h \}, \\
V_h &= \{ \tilde{z}_h \in L^2(\Omega)^2 : \tilde{\nabla} \tilde{z}_h \in L^2(\Omega); \quad \tilde{z}_h|_K \in (P_1)^2, \quad \tilde{z}_h|_{\partial K} \in P_0, \quad \forall K \in \tau_h; \quad \tilde{z}_h|_{\Gamma - \Gamma_0} = 0 \}, \\
W_h &= \{ y_h \in L^2(\Omega) : y_h|_K \in P_1, \quad \forall K \in \tau_h; \quad y_h|_{\Gamma - \Gamma_0} = 0 \}.
\end{align*}
\]

**Remark 1.** For instance, if we restrict to the reference triangle with vertices \((0, 0), (1, 0)\) and \((0, 1)\), the functions of \(V_h\) will be in the three-dimensional vector space spanned by the functions \(v^1(x_1, x_2) = (x_1, -1 + x_2), \quad v^2(x_1, x_2) = \sqrt{2}x_1, \quad v^3(x_1, x_2) = \sqrt{2}x_2\) and \(v^4(x_1, x_2) = (-1 + x_1, x_2)\). For any other triangle \(K\) in \(\tau_h\) it is necessary the usual affine transformation.

We must recall that functions in \(V_h\) are discontinuous, but their normal components are continuous and constant on the edges of the triangles. In fact, they are taken as degrees of freedom.
Then, we choose the fully discretized approximation of the adjoint system

\[
p_h = 0,
\]
\[
\bar{w}_h = 0,
\]
\[
s_h = 0,
\]
for \(n = N - 1, \ldots, 0:\)

\[
(p_h, \bar{w}_h, s_h) \in U_h \times V_h \times W_h \text{ such that }
\]
\[
\int_{\Omega} \frac{p_h - p_{h+1}}{\Delta t} \cdot r_h = 0, \quad \forall r_h \in U_h,
\]
\[
\int_{\Omega} \frac{\bar{w}_h - \bar{w}_{h+1}}{\Delta t} \cdot \bar{z}_h + \int_{\Omega} (\bar{w}_h \cdot \nabla \bar{z}_h) + \int_{\Omega} \frac{\bar{w}_h \cdot (\bar{u}_h \cdot \nabla \bar{z}_h)}{\Delta t} = 0, \quad \forall \bar{z}_h \in V_h,
\]
\[
\int_{\Omega} \frac{s_h - s_{h+1}}{\Delta t} \cdot y_h + \int_{\Omega} \bar{w}_h \cdot \nabla s_h y_h + \int_{\Omega} s_h \bar{u}_h \cdot \nabla y_h + k \int_{\Omega} s_h y_h
\]
\[
+ \beta \int_{\Omega} \nabla s_h \cdot \nabla y_h + n \int_{\Omega} \chi_A(\rho_h - c)_+ y_h = 0, \quad \forall y_h \in W_h,
\]

where \((H^n_h, \bar{u}^n_h, \rho^n_h)\) is a discretized solution of the state system (5) obtained by a characteristics-mixed finite element method similar to the one introduced here for the adjoint system (see, for instance, [5] and [2]), and \(Y_{h+1}^{n+1}\) is an approximation of \(Y^{n+1}\) computed by using the forward Euler scheme, that is,

\[
Y_{h+1}^{n+1}(x) = x + \Delta t \bar{u}_h^n(x).
\]

Finally, taking into account the expression obtained in Theorem 1 for the derivative

\[
DJ(q)(\delta) = \int_0^T \int_{\Gamma^-} [m \eta^2 q + \eta p + v(\nabla \bar{w})] \delta,
\]
we can obtain this approximation of the cost gradient

\[
DJ_h^\Delta (q^\Delta_h) = m\Delta t \sum_{n=0}^{N-1} \int_{I^-} (\eta_{h}^{n+1})^2 q_h^{n+1} \delta_h^{n+1} \\
+ \Delta t \left[ \sum_{n=0}^{N-1} \int_{I^-} \eta_{h}^{n+1} p_h^{n+1} \delta_h^{n+1} + v \sum_{n=0}^{N-1} \int_{I^-} (\nabla \cdot w_h^{n+1}) \delta_h^{n+1} \right], \quad \forall q^\Delta_h, \delta_h \in U_{ad,h}.
\] (12)

**Remark 2.** It is also possible to present an alternative scheme consisting of the discrete (not the discretized) adjoint system: we can introduce discretizations of the state system and the cost function (but not for the adjoint system and the cost gradient). In fact, once the discretizations for state and cost are chosen, these yield an unique discrete adjoint system which will provides us with an expression for the exact gradient of the discretized cost function (usually different from the previously obtained approximation (12) for the cost gradient). This alternative approach will be addressed by the authors in a forthcoming paper.

5. Numerical resolution

To solve the discrete control problem \((\mathscr{P}_h^\Delta)\) we propose the use of a limited-memory BFGS algorithm [10,11] for bound constrained optimization problems. By numerical reasons, we will solve the following equivalent problem, where we have included an additional lower bound (actually related to technological constraints on the velocity of injected clear water, which may not surpass a critical threshold)

\[
(\mathscr{P}_h^\Delta) \min_{q_h^\Delta \in \tilde{U}_{ad,h}^\Delta} J_h^\Delta (q_h^\Delta),
\]

where

\[
\tilde{U}_{ad,h}^\Delta = \{ l_h \in L^2(I^-) : l_h|_{\partial K \cap I^-} \in P_0, \forall K \in \tau_h; \ 0 \geq l_h \geq -Q \}^N
\]

for \(Q\) large enough.

If we consider \(a_m, \ m = 1, \ldots, M\), the \(M\) nodes of the triangulation \(\tau_h\) lying on the boundary \(I^-\), and we denote by

\[
Q_h^\Delta = \{ Q^m_n \}_{m=1, \ldots, M, \ n=1, \ldots, N} \in \mathbb{R}^{M \times N},
\]

where \(Q^m_n = q_h^n(a_m)\), the discrete control problem can be written in the form

\[
(\mathscr{P}_h^\Delta) \min_{Q_h^\Delta \in [-Q,0]^{M \times N}} \hat{J}_h^\Delta (Q_h^\Delta)
\]

for the new cost function \(\hat{J}_h^\Delta\) defined by \(\hat{J}_h^\Delta (Q_h^\Delta) = J_h^\Delta (q_h^\Delta)\).

The algorithm can be easily summarized in the following way: starting from an initial admissible vector \(Q_h^\Delta (0)\), we construct a sequence of iterates \(Q_h^\Delta (k+1), \ k = 0, 1, 2, \ldots, \) by the recursive formula

\[
Q_h^\Delta (k+1) = H(Q_h^\Delta (k) - z_k \ D_k \ \hat{J}_h^\Delta (Q_h^\Delta (k))),
\]
where for all vector $\mathbf{Z}_h^{\Delta t} = \{Z^n_m\} \in \mathbb{R}^{M \times N}$ we denote by $\Pi(Z_h^{\Delta t}) = \{\Pi^n_m\} \in [-Q, 0]^{M \times N}$ the projected vector with coordinates

$$
\Pi^n_m = \begin{cases} 
0 & \text{if } Z^n_m \geq 0, \\
Z^n_m & \text{if } 0 > Z^n_m > -Q, \\
-Q & \text{if } -Q \geq Z^n_m;
\end{cases}
$$

$\alpha_k$ is chosen by the Armijo rule [11], and $D_k$ is an adequately chosen positive definite matrix (see, for instance, [6] and the references therein). The discrete gradient $\nabla J_h^{\Delta t}(Q_h^{\Delta t}(k))$ can be easily obtained from expression (12). The convergence test is based on the norm of the cost gradient with respect to the nonactive variables and on the difference between two consecutive iterates. In case of stopping, the algorithm converges to a solution of the discrete control problem ($\hat{\mathcal{P}}_h^{\Delta t}$).

For the numerical experiments we have considered the following situation, depicted in Fig. 1: the bay $\Omega$, whose dimensions are about $10 \times 5$ km, is occupied by shallow water and the contaminants are dumped into the sea, through $L = 1$ submarine outfall located at point $b_1$, with constant rate $m_1 = 10^8$ u/s. In order to purify the protected area $A_1$ (in white in the picture) we inject clear water through the boundary $\Gamma^-$. We assume that the time interval $[0, 3600]$ is divided into $N = 20$ equal intervals ($\Delta t = 180$ s). For the discretization of $\Omega$ we use a mesh of 860 elements, where only $M = 1$ node lies over the boundary $\Gamma^-$. For the discretization of $\Gamma^-$ (namely, the midpoint of the only edge). In this node, the height of water is assumed to be $\eta = 1$ meter; in the open sea the boundary condition over the height of water is a wave-like function. We consider a fixed threshold $c = 7000$ u/m$^3$ for the coliphorm concentration.
The algorithm has been developed for a lower bound given by \( Q = 10^4 \). Starting from an initial normal velocity with constant value \( Q^h_{\text{A}}(0) = 15 \), we obtain convergence in nine iterations. Fig. 2 shows the optimal normal velocity achieved by the algorithm.

6. Conclusions

In this work the authors have formulated, analyzed and solved an optimal control problem related to the purification of polluted areas of shallow water by the injection of clear water through a small portion of the boundary. Once the ecological problem is mathematically well posed, a formal optimality condition is obtained for the characterization of its solutions. A limited-memory BFGS algorithm for bound constrained optimization problems is proposed for the numerical resolution, where the gradient of the cost function can be computed by means of the discretized adjoint system. Finally, the good performance of the algorithm is confirmed by the numerical experiments developed by the authors.

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