11th World Congress on Computational Mechanics (WCCM XI)
5th European Conference on Computational Mechanics (ECCM V)
6th European Conference on Computational Fluid Dynamics (ECFD VI)
E. Oñate, J. Oliver and A. Huerta (Eds)

CONTROLLING EUTROPHICATION IN A MOVING DOMAIN

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Key words: Eutrophication, Optimal control, Moving domain

Abstract. This paper studies the environmental problem related to controlling eutrophication inside a sensitive zone, through a regulation of the wastewater discharges in the region. After presenting a detailed mathematical formulation of the optimal control problem posed on a free-boundary moving domain, we introduce some theoretical results on existence-regularity of optimal solutions, and their characterization by a first order optimality system. In the last part of the paper a numerical algorithm for the practical resolution of the control problem is proposed, and some numerical tests are also given.

1 INTRODUCTION

Eutrophication is an environmental process whereby large water bodies (lakes, estuaries, slow-moving streams, and so on) receive an excess of nutrients (nitrogen and/or phosphorus) that stimulate excessive undesirable plant growth (mainly, algae). This enhanced plant growth, usually known as an algal bloom, reduces dissolved oxygen in the water when dead plant material decomposes and can cause other organisms (fish, shellfish, seabirds, and even small mammals) to die, leading to changes in animal and plant populations and degradation of water and habitat quality. Nutrients come from many sources, such as fertilizers applied to agricultural fields, golf courses, and suburban lawns; deposition of nitrogen from the atmosphere; phosphate detergents; erosion of soil containing nutrients; and sewage treatment plant discharges.

In the present paper we are interested in controlling the eutrophication processes along a time interval $I = (0, T)$ inside a sensitive zone from a large water body $\Omega(t)$, where a wastewater outfall discharges polluted water with a high concentration of nutrients, coming, for instance, from a sewage treatment plant. In particular, we try to keep the level of eutrophication inside this zone $G(t) \subset \Omega(t)$ under safety thresholds, and with an economic cost (due to wastewater purification processes) as low as possible. From a mathematical viewpoint, the problem $(\mathcal{P})$ related to controlling eutrophication along a time interval I in a moving domain $\Omega(t)$ can be formulated as an optimal control problem with state and control constraints.

Eutrophication can be modelled by a system of partial differential equations, commonly presenting a high complexity due to the great variety of phenomena appearing on it. In this paper we have considered a simplified - but realistic - model, where only five biological species appear. So, we consider the variable $\mathbf{u} = (u^1, \ldots, u^5)$, where u^1 represents a generic nutrient concentration (usually nitrogen and/or phosphorus), u^2 the phytoplankton concentration, u^3 the zooplankton concentration, u^4 the organic detritus concentration, and u^5 the dissolved oxygen concentration. The evolution of these five species into a moving water domain $\Omega(t) \subset \mathbb{R}^3$ for a time interval I, can be described by the system of coupled nonlinear partial differential equations for advection-diffusion-reaction with Michaelis-Menten kinetics presented by the authors in the recent paper [1], where the moving domain problem has been analyzed from an ALE perspective. The source term corresponding to the wastewater outfall is modelled with a Dirac measure $g(t)\delta(x-b)$, where $g(t)$ represents the pollutant concentration (nitrogen and/or phosphorus in our case) discharged through the outfall, and b is the outfall location.

Moreover, we impose some technological constraints on the control g (related, for instance, to lower and upper bounds corresponding to the purification capacities of the sewage treatment plant: higher levels of purification lead to lower pollutant discharges). In this way, we assume that the control $g \in \mathcal{U}_{ad}$, a convex, closed, bounded subset of $L^2(0, T)$. We also impose several state constraints, aimed to guarantee the quality of water inside the sensitive zone $G(t)$ all along the time interval I. So, we need to assure that the averaged concentrations of the five species remain between some desired thresholds η^i and τ^i (respectively, the lower and upper bounds for species $i \in \{1, \ldots, 5\}$ in the sensitive zone).

Finally, from a realistic viewpoint, we are interested in reducing the global economic cost of the purification process, i.e., minimizing the cost function $J(g) = \int_0^T m(g(t))dt$, where function $m(g)$ denotes the cost of the depuration in the treatment plant. Summarizing, the control and state constrained optimal control problem $(\mathcal{P})$ we are interested in consists of minimizing the cost function J such that the control g verifies the control constraints, and the state $\mathbf{u}$ satisfies the state constraints.

In a first part of the paper, we present several theoretical results on existence-regularity of optimal solutions, and their characterization by a first order optimality system. In the second part of the work a complete numerical algorithm for the resolution of the control problem is proposed, and several numerical results are also given. This numerical algorithm combines scientific software Freefem++ [5] (for the numerical resolution of the hydrodynamic equations and the state system) interfaced with interior point algorithm IPOPT [7] (for the resolution of the nonlinear constrained optimization problem, obtained from the space-time discretization of the continuous control problem).

2 MATHEMATICAL FORMULATION OF THE PROBLEM

As a first step in order to control eutrophication, we need to model the interactions between the different species taking part in the process. Eutrophication can be modelled by a system of partial differential equations, commonly presenting a high complexity due to the great variety of phenomena appearing on it. In this paper we have considered a simplified - but realistic - model, where only five biological species appear (the specific formulation of biochemical interaction terms and their meaning can be seen, for instance, in Canale [4]). So, we consider the variable $\mathbf{u} = (u^1, \ldots, u^5)$, where u^1 represents a generic nutrient concentration (usually nitrogen and/or phosphorus), u^2 the phytoplankton concentration, u^3 the zooplankton concentration, u^4 the organic detritus concentration, and u^5 the dissolved oxygen concentration. The evolution of these five species into a moving water domain $\Omega(t) \subset \mathbb{R}^3$ (and with a smooth enough boundary $\partial\Omega(t)$), for a time interval I, can be described by the following system of coupled nonlinear partial differential equations for advection-diffusion-reaction with Michaelis-Menten kinetics:

$$\left\{ \begin{array}{ll} \dfrac{\partial u^i}{\partial t} + \nabla_x u^i \cdot \mathbf{v} - \mathrm{div}_x(\mu^i \nabla_x u^i) - A^i(t,x,\mathbf{u}) = g^i & \text{in } \ \Omega(t),\ t \in I, \\ \mu^i \nabla_x u^i \cdot \mathbf{n} + \alpha^i (u^i - h^i) = 0 & \text{on } \ \partial\Omega(t),\ t \in I, \\ u^i(0) = u_0^i & \text{in } \ \Omega(0), \end{array} \right. \tag{1}$$

for $i = 1, \ldots, 5$, where $\mathbf{n}$ represents the outward unit normal vector, and where the reaction term $\mathbf{A} = (A^i) : \cup_{t \in I}\{t\} \times \Omega(t) \times [\mathbb{R}_+]^5 \longrightarrow \mathbb{R}^5$ is given by the following nonlinear expression:

$$\mathbf{A}(t,x,\mathbf{u}) = \left(\begin{array}{c} -C_{nc}\left(L(t,x)\dfrac{u^1}{K_N + u^1}u^2 - K_r u^2 \right) + C_{nc}K_{rd}\Theta^{\theta(t,x)-20}u^4 \\ L(t,x)\dfrac{u^1}{K_N + u^1}u^2 - K_r u^2 - K_{mf}u^2 - K_z \dfrac{u^2}{K_F + u^2}u^3 \\ C_{fz}K_z \dfrac{u^2}{K_F + u^2}u^3 - K_{mz}u^3 \\ K_{mf}u^2 + K_{mz}u^3 - K_{rd}\Theta^{\theta(t,x)-20}u^4 \\ C_{oc}\left(L(t,x)\dfrac{u^1}{K_N + u^1}u^2 - K_r u^2 \right) - C_{oc}K_{rd}\Theta^{\theta(t,x)-20}u^4 \end{array} \right) \tag{2}$$

where $\mathbf{v}$ represents the water velocity; $\mu_i,\ i = 1, \ldots, 5$, are the diffusion coefficients of each species; C_{nc} is the nitrogen-carbon stoichiometric relation; L is the luminosity function, given by relation:

$$L(t,x,u^2) = \mu C_t^{\theta(t,x)-20} \frac{I_0}{I_s} e^{-(\phi_1+\phi_2 u^2)x_3}, \tag{3}$$

with μ the maximum phytoplankton growth rate, C_t the phytoplankton growth thermic constant, θ the water temperature, I_0 the incident light intensity, I_s the light saturation, ϕ_1 the light absorption by water, and ϕ_2 the light absorption by phytoplankton; K_N is the nitrogen half-saturation constant; K_{rd} is the detritus regeneration rate; Θ is the detritus regeneration thermic constant; K_r is the phytoplankton endogenous respiration rate; K_{mf} is the phytoplankton death rate; K_z is the zooplankton predation (grazing); K_F is the phytoplankton half-saturation constant; C_{fz} is the grazing efficiency factor; K_{mz} is the zooplankton death rate (including predation); W_{fd} is the falling velocity of organic detritus; and C_{oc} is the oxygen-carbon stoichiometric relation.

Finally, terms g^i, u_0^i, h^i, and α^i, for $i = 1, \ldots, 5$, stand, respectively, for source terms distributed in the domain (that will be the control in our problem), initial concentrations, Robin boundary coefficients, and mass flow coefficients through the boundary $\partial\Omega(t)$. For the sake of completeness, we consider this boundary split into four parts $\partial\Omega(t) = \partial\Omega_1(t)\cup\partial\Omega_2(t)\cup\partial\Omega_3(t)\cup\partial\Omega_4(t)$, where $\partial\Omega_1(t)$ corresponds to the open boundary, $\partial\Omega_2(t)$ to the upper surface (free boundary), $\partial\Omega_3(t)$ to the coast, and $\partial\Omega_4(t)$ to the bottom.

The classical system of Navier-Stokes equations (within the standard ALE framework [6]) will be used to model hydrodynamics:

$$\left\{ \begin{array}{ll} \dfrac{\partial \mathbf{v}}{\partial t} + \nabla_x \mathbf{v}\, \mathbf{v} - \mathrm{div}_x(\nu \nabla_x \mathbf{v}) + \nabla_x^T p = \mathbf{f} & \text{in } \ \Omega(t),\ t \in I \\ \mathrm{div}_x(\mathbf{v}) = 0 & \text{in } \ \Omega(t),\ t \in I \\ \mathbf{v} = \mathbf{v}_{in} & \text{on } \ \partial\Omega_1(t),\ t \in I, \\ \sigma \mathbf{n} = 0 & \text{on } \ \partial\Omega_2(t),\ t \in I, \\ \sigma \mathbf{n}\cdot\tau = 0, \quad \mathbf{v}\cdot\mathbf{n} = 0 & \text{on } \ \partial\Omega_3(t)\cup\partial\Omega_4(t),\ t \in I, \\ \mathbf{v}(0) = \mathbf{v}_0 & \text{in } \ \Omega(0), \end{array} \right. \tag{4}$$

where, $\mathbf{v}$, p and $\mathbf{f}$ denote, respectively the fluid velocity, the pressure and the body forces, ν is the coefficient of dynamic viscosity, $\mathbf{v}_0$ represents the initial velocity, $\mathbf{v}_{in}$ is the velocity of fluid on the open boundary $\partial\Omega_1$, and $\sigma = -pI + \nu\left(\nabla_x \mathbf{v} + \nabla_x^T \mathbf{v}\right)$ stands for the stress tensor.

In previous works of the authors, the source term corresponding to the wastewater outfall was modelled *via* a Dirac measure $g(t)\delta(x-\mathbf{b})$, where $g(t)$ represents the pollutant concentration (nitrogen and/or phosphorus in our case) discharged through the outfall, and $\mathbf{b}$ is the outfall location. However, in this work, in order to simplify the problem, we have chosen a regularization of the Dirac distribution, based on the following sequence of smooth, compact support functions:

$$\varphi_{\mathbf{b},\epsilon}(x) = \left\{ \begin{array}{ll} e^{\frac{1}{\|x-\mathbf{b}\|^2-\epsilon^2}} & \text{if } \|x-\mathbf{b}\| < \epsilon, \\ 0 & \text{if } \|x-\mathbf{b}\| \geq \epsilon, \end{array} \right. \tag{5}$$

which converges, as ϵ goes to zero, to the Dirac measure $\delta(x-\mathbf{b})$ in the sense of distributions. To be exact, we will model the source term for nutrients g^1 in system (1) as $R_{\mathbf{b},\epsilon}(g)=g(t)\varphi_{\mathbf{b},\epsilon}(x)$, where $g(t)$ represents the load of nutrients discharged through the outfall at each time $t\in I$, $\mathbf{b}$ gives the outfall location, and parameter ϵ will be determined from the mesh size. The other source terms $g^2,\ldots,g^5$ will be considered null, since no other species (but nutrients) are discharged from the wastewater outfall. Thus, the source terms in (1) will be given by

$$g^i=\delta_{i,1}\,R_{\mathbf{b},\epsilon}(g) \tag{6}$$

where $\delta_{i,j}$ represents the Kronecker delta.

Moreover, we need to impose some technological constraints on the control g (related, for instance, to lower and upper bounds corresponding to the purification capacities of the sewage treatment plant: higher levels of purification lead to lower pollutant discharges). In this way, we assume that the control g belongs to a convex, closed, bounded subset $\mathcal{U}_{ad}$ of $L^2(0,T)$, that is, we consider the following control constraint:

$$g\in\mathcal{U}_{ad}. \tag{7}$$

On the other hand, we also impose several state constraints, aimed to guarantee the quality of water inside the sensitive zone $G(t)$ all along the time interval I. So, we need to assure that the averaged concentrations of the five species remain between some desired thresholds:

$$\eta^i\le\frac{1}{\|G(t)\|}\int_{G(t)}u^i(t,x)\,dx\le\tau^i,\quad\forall t\in I,\quad\forall i=1,\ldots,5, \tag{8}$$

where η^i and τ^i denote, respectively, the lower and upper bounds for each one of the species in the sensitive zone, and $\|G(t)\|$ represents the volume occupied by domain $G(t)$ at time $t\in I$.

Finally, from a realistic viewpoint, we are interested in reducing the global economic cost of the purification process, i.e., minimizing the cost function:

$$J(g)=\int_0^T m(g(t))dt, \tag{9}$$

where function $m(g)$ denotes the cost of the depuration in the treatment plant. This function m depends on the pollutant discharge in such a way that a lower level of discharge leads to a more intensive depuration and, consequently, to a higher cost, and takes into account that absolute depuration is not feasible and that there exists a minimum cost, even in the case when no treatment is developed.

Summarizing, the control and state constrained optimal control problem $(\mathcal{P})$ we are interested in consists of minimizing the cost function (9) such that the control g verifies the control constraint (7), and the state $\mathbf{u}$ - solution of system (1) with source terms given by (6) - satisfies the state constraints (8).

3 THE OPTIMAL CONTROL PROBLEM

This section is initially concerned with the analysis (study of the existence and uniqueness of solution) of the state system (1) related to eutrophication model. In [3] and [1] the authors analyze the existence of solution for this type of state systems, for the respective cases of fixed and moving domains. In order to demonstrate these existence results it is necessary to impose some additional hypotheses on the regularity of the ALE mapping Y and the fluid velocity $\mathbf{v}$.

For the variational formulation of the state system we need to introduce the following functional spaces:

$$W(\Omega(t)) = \left\{ u \in L^2(I; H^1(\Omega(t))) \ : \ \frac{du}{dt} \in \left(L^2(I; H^1(\Omega(t)))\right)' \right\},$$
$$V(\Omega(t)) = \left\{ \psi : \cup_{t\in I}\{t\} \times \Omega(t) \to \mathbb{R} \ : \ \psi = \widehat{\psi} \circ Y(t,\cdot)^{-1}, \text{ with } \widehat{\psi} \in H^1(\widehat{\Omega}) \right\}.$$

All along this section we will assume that, for each $t \in I$, the domain $\Omega(t) = Y(t, \widehat{\Omega})$ is bounded with boundary $\partial\Omega(t)$ Lipschitz-continuous, and that the fluid velocity is such that $\mathbf{v} \in [L^\infty(I; W^{1,\infty}(\Omega(t)))]^3$.

In later argumentations, stronger smoothness assumptions will be necessary on the regularity of the ALE mapping Y. We will introduce two possibilities depending on the desired regularity for the solution of the state system:

[H1] $Y \in [W^{1,\infty}(I; W^{1,\infty}(\widehat{\Omega}))]^3$, with inverse $Y^{-1} \in [W^{1,\infty}(I; W^{1,\infty}(\Omega(t)))]^3$.

[H2] $Y \in [W^{1,\infty}(I; W^{2,\infty}(\widehat{\Omega}))]^3$, with inverse $Y^{-1} \in [W^{1,\infty}(I; W^{2,\infty}(\Omega(t)))]^3$.

Under above hypotheses, we can obtain several results on existence, uniqueness and regularity for the solution of the state system (1). The main one is related to the case of the weaker hypothesis [H1], and its proof can be seen in the early paper of the authors [1, Theorem 15]:

Theorem 1: *Under the general hypothesis [H1] and the following additional assumptions on the data for the state system:*

- $g^i \in L^2(I; L^2(\Omega(t))),\ \forall i = 1,\ldots,5,$ *such that:*
  - * $0 \le g^i(t,x) \le M,$ *a.e.* $x \in \Omega(t),\ t \in I,\ \forall i = 1,\ldots,4,$
  - * $|g^5(t,x)| \le M,$ *a.e.* $x \in \Omega(t),\ t \in I,$
- $u_0^i \in L^2(\Omega(0)),\ \forall i = 1,\ldots,5,$ *such that:*
  - * $0 \le u_0^i(x) \le M,$ *a.e.* $x \in \Omega(0),\ \forall i = 1,\ldots,4,$
  - * $|u_0^5(x)| \le M,$ *a.e.* $x \in \Omega(0),$

then there exists a unique weak solution $\mathbf{u} \in [W(\Omega(t)) \cap L^\infty(I; L^2(\Omega(t)))]^5$ *of the state system (1) satisfying:*

- $\|\mathbf{u}\|_{[W(\Omega(t))\cap L^\infty(I;L^2(\Omega(t)))]^5} \leq C(T,M)$
- $0 \leq u^i(t,x) \leq C(T,M),$ *a.e.* $x \in \Omega(t),\ t \in I,\ \forall i = 1,\ldots,4,$
- $|u^5(t,x)| \leq C(T,M),$ *a.e.* $x \in \Omega(t),\ t \in I.$

For the case of stronger hypotheses we have the following result:

Theorem 2: *If we also assume that hypothesis [H2] is satisfied and that initial datum is such that* $\mathbf{u}_0 \in [W^{2-\frac{2}{q},q}(\Omega(0))]^5$ *with* $q > 5/2$*, then the state system admits a unique solution* $\mathbf{u} \in [L^q(I; W^{2,q}(\Omega(t))) \cap W^{1,q}(I; L^q(\Omega(t))) \cap \mathcal{C}(\overline{\cup_{t\in I}\{t\} \times \Omega(t)})]^5$*, that verifies the estimate:*

$$\|\mathbf{u}\|_{[L^q(I;W^{2,q}(\Omega(t)))\cap W^{1,q}(I;L^q(\Omega(t)))\cap\mathcal{C}(\overline{\cup_{t\in I}\{t\}\times\Omega(t)})]^5} \leq C\left(T, M, \|\mathbf{u}_0\|_{[W^{2-\frac{2}{q},q}(\Omega(0))]^5}\right).$$

3.1 Characterization of the optimal solutions

In this subsection we will envisage the existence and characterization of solutions for the control problem $(\mathcal{P})$, whose complete proofs can be seen in [2]:

Theorem 3: *Let us assume that hypothesis [H1] is verified, and also that the admissible set* $\mathcal{U}_{ad} \subset \{g \in L^2(I)\ :\ 0 \leq g(t) \leq M,\ a.e.\ t \in I\}$ *is convex, closed and bounded, the function* $m : [0,M] \subset \mathbb{R} \longrightarrow \mathbb{R}$ *is continuous, and the set of feasible controls is nonempty. Then, the optimal control problem* $(\mathcal{P})$ *admits, at least, a solution.*

Now, we can prove the following optimality result for the control problem:

Theorem 4: *Under the general hypothesis of Theorem 1, we also assume that the hypothesis [H2] is verified, the function* $m : L^2(I) \to \mathbb{R}$ *is differentiable, and the initial data are such that* $\mathbf{u}_0 \in [W^{2-\frac{2}{q},q}(\Omega(0))]^5$*, with* $q > 5/2$*. Let* $\tilde{\rho} \in \mathcal{U}_{ad}$ *be a solution of the control problem* $(\mathcal{P})$*, with associated state* $\mathbf{u}_{\tilde{\rho}}$ *in the space* $[L^q(I; W^{2,q}(\Omega(t))) \cap W^{1,q}(I; L^q(\Omega(t))) \cap \mathcal{C}(\overline{\cup_{t\in I}\{t\} \times \Omega(t)})]^5$*. Then, there exist elements* $\gamma \geq 0$ *and* $\lambda^i \in M(\bar{I})$*,* $i = 1,\ldots,5$*, such that:*

$$\gamma + \sum_{i=1}^{5} \|\lambda^i\|_{M(\bar{I})} > 0, \tag{10}$$

$$\sum_{i=1}^{5} \langle \lambda_i, g^i - \frac{1}{\|G(t)\|} \int_{G(t)} u^i_{\tilde{\rho}}\, dx \rangle_{M(\bar{I}),\mathcal{C}(\bar{I})} \leq 0, \quad \forall \mathbf{g} \in E, \tag{11}$$

satisfying the following optimality condition:

$$\gamma \int_0^T m'(\widetilde{\rho})(\rho - \widetilde{\rho})dt + \int_0^T \int_{\Omega(t)} R_{\mathbf{b},\epsilon}(\rho - \widetilde{\rho}) q^1 \, dxdt \leq 0, \quad \forall \rho \in \mathcal{U}_{ad} \tag{12}$$

with $\mathbf{q} \in [L^2(I; H^1(\Omega(t))) \cap L^\infty(I; L^2(\Omega(t)))]^5$ *the unique solution of the adjoint system:*

$$\begin{aligned} &\int_0^T \int_{\Omega(t)} \left\{ \frac{\partial \psi}{\partial t} + (\mathbf{v} - \mathbf{w}) \cdot \nabla_x^T \psi + div_x(\nabla_x \psi) \right\} q^i \, dxdt = \\ &\qquad \int_0^T \int_{\Omega(t)} [D_{\mathbf{u}} A(\mathbf{u}_{\widetilde{\rho}})^T \mathbf{q}]_i \psi \, dxdt + \int_0^T \left(\frac{1}{\|G(t)\|} \int_{G(t)} \psi \, dx \right) d\lambda^i, \quad \forall \psi \in \mathcal{R}, \end{aligned} \tag{13}$$

where

$$\mathcal{R} = \Big\{ \widehat{\psi} \in \mathcal{C}(\overline{\cup_{t \in I} \{t\} \times \Omega(t)}) \cap L^2(I; H^1(\Omega(t))) \ : \ \frac{\partial \psi}{\partial t} + A\psi \in L^\infty(\cup_{t\in I} \{t\} \times \Omega(t)),$$
$$\partial_{\mathbf{n}_{A^*}} \psi = 0 \ \text{on} \ \cup_{t\in I} \{t\} \times \partial\Omega(t), \quad \psi(0) = 0 \ \text{in} \ \Omega(0) \Big\}.$$

4 NUMERICAL RESOLUTION OF THE CONTROL PROBLEM

In order to obtain the numerical solution of the control problem, we will proceed to a full discretization of the problem $(\mathcal{P})$. The space semi-discretization will be done by the well-known method of finite elements, so it will not be detailed here. Thus, we will focus our attention on the time semi-discretization, that uses the partition $\{t_0, t_1, \ldots, t_N\}$ of the time interval I for a time step $\Delta t = T/N$. So, we consider the following time discretization for the different elements conforming the optimal control problem:

- Discretization of the space of admissible controls:

$$\mathcal{U}_{ad}^{\Delta t} = \left\{ \rho \in \mathbb{R}^N \ : \ N_{min} \leq \rho_n \leq N_{max}, \ \forall n = 1, \ldots, N \right\}, \tag{14}$$

  where N_{min} and N_{max} represent, respectively, allowed minimal and maximal discharges.

- Discretization of the cost functional:

$$F^{\Delta t}(\rho) = \sum_{n=1}^{N} m(\rho_n). \tag{15}$$

- Discretization of the state system:

$$\left\{\begin{array}{l} u_0^i \in H^1(\Omega(0)),\ i=1,\ldots,5, \text{ given.} \\ \text{For } n=0,\ldots,N-1,\ u_{n+1}^i \in H^1(\Omega(t_n)),\ i=1,\ldots,5, \text{ is the solution of:} \\ \alpha \int_{\Omega(t_n)} u_{n+1}^i z\,dx + \int_{\Omega(t_n)} \mu_i \nabla_x u_{n+1}^i \cdot \nabla_x z\,dx dx = \int_{\Omega(t_n)} A_{n+1}^i(\mathbf{u}_{n+1}) z dx \\ \quad + \int_{\Omega(t_n)} \delta_{i,1} R_{\mathbf{b},\epsilon}(\rho_{n+1}) z\,dx + \alpha \int_{\Omega(t_n)} u_n^i(X_{\mathbf{r}_n}(t_n)) z\,dx, \\ \quad \forall z \in H^1(\Omega(t_n)), \quad i=1,\ldots,5. \end{array}\right. \tag{16}$$

- Discretization of the state constraints: If we introduce the function

$$\mathbf{G} : \rho \in \mathcal{U}_{ad}^{\Delta t} \longrightarrow \mathbf{G}(\rho) = [\mathbf{G}_1(\rho), \mathbf{G}_2(\rho), \ldots, \mathbf{G}_N(\rho)]^T \in \mathbb{R}^{N\times 5}$$

where, for any $n=1,\ldots,N$,

$$\mathbf{G}_n(\rho) = \frac{1}{\|G(t_n)\|}\left(\int_{G(t_n)} u_n^1\,dx,\ \int_{G(t_n)} u_n^2\,dx,\ \int_{G(t_n)} u_n^3\,dx,\ \int_{G(t_n)} u_n^4\,dx,\ \int_{G(t_n)} u_n^5\,dx\right)^T,$$

then the state constraints

$$\eta^i \leq \frac{1}{\|G(t_n)\|}\int_{G(t_n)} u_n^i\,dx \leq \tau^i,\ \forall n=1,\ldots,N,\ \forall i=1,\ldots,5,$$

can be rewritten in an equivalent way as $\mathbf{G}(\rho) \in E^{\Delta t}$, with

$$E^{\Delta t} = \left\{\mathbf{g} \in \mathbb{R}^{N\times 5}\ :\ \eta^i \leq g_n^i \leq \tau^i,\ \forall n=1,\ldots,N,\ \forall i=1,\ldots,5\right\},$$

Thus, taking this into account, the discretized optimal control problem reads now as:

$$(\mathcal{P}^{\Delta t}) \qquad \text{minimize } F^{\Delta t}(\rho) \text{ such that } \rho \in \mathcal{U}_{ad}^{\Delta t} \text{ and } \mathbf{G}(\rho) \in E^{\Delta t}$$

Once discretized the control problem, we are led to solve the constrained optimization problem $(\mathcal{P}^{\Delta t})$. In order to do this, we will use an interior point algorithm. The use of this type of methods requires at each iteration, in addition to the usual computation of the cost function and of the constraints, the evaluation of the gradients of the cost function (which is straightforward in our case) and of the Jacobian matrix for the constraints (which is a much more complex task).

5 NUMERICAL RESULTS

Although we have developed a large number of numerical examples, we will show here only one of them. Moreover, in order to present the graphical results in a simpler way, this example will correspond to a two-dimensional material domain. So, for our example

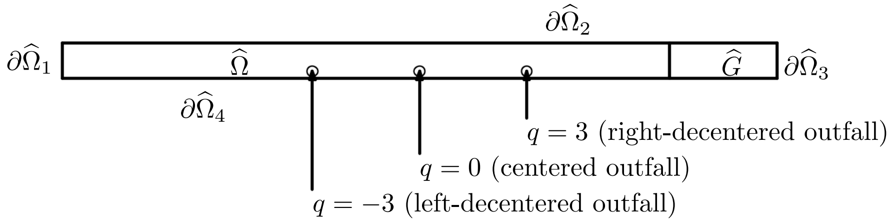

Figure 1: Reference domain $\widehat{\Omega}$ for numerical experiences, showing the boundaries $\partial\widehat{\Omega}_j,\ j = 1, \ldots, 4$, the sensitive zone $\widehat{G} \subset \widehat{\Omega}$, and the respective outfall locations for the three numerical tests.

we have taken a time interval of $T = 48$ hours, and as the reference domain the rectangle $\widehat{\Omega} = (-100, 100) \times (0, 10) \subset \mathbb{R}^2$ with a control domain given by $\widehat{G} = (70, 100) \times (0, 10) \subset \widehat{\Omega}$. (These domains, and the corresponding boundaries, can be seen in Fig. 1. We can also observe here the three different locations for the wastewater outfalls corresponding to the three scenarios under study).

For the finite element space discretization we have considered a $\mathcal{P}_2 - \mathcal{P}_1$ method for the hydrodynamic model, and a $\mathcal{P}_1$ method for the state system. These space discretizations have been implemented in the scientific software Freefem++ [5], employing for the reference domain $\widehat{\Omega}$ a regular triangular mesh of 800 elements (right triangles of base length $2.5\,m$ and height $2\,m$).

Finally, the numerical resolution of the nonlinear constrained optimization problem (obtained from the space-time discretization of the continuous control problem) has been developed with the help of the interior point algorithm IPOPT [7], interfaced with Freefem++.

In order to show the influence of the outfall location in the optimal results, we present here three numerical examples corresponding to three different locations $\mathbf{b}$ of the wastewater outfall (as given in Fig. 1), considering points of the form $\mathbf{b} = (q, 2)$, where q can take the three possible values:

- $q = -3$ (left-decentered outfall),
- $q = 0$ (centered outfall),
- $q = 3$ (right-decentered outfall).

In all these tests we have chosen an initial (time-constant) control corresponding to $g(t, x) = 1.0 \times 10^{-3}$ for the iterative optimization algorithm.

So, in Fig. 2 we can see the optimal controls achieved for the three numerical examples. We observe the strong influence of the outfall location on the optimal discharges: the farer the outfall is to the protected zone $\tilde{G}$, the higher the allowed discharge of pollution. We can also note in Fig. 2 the "periodic" behaviour of the solution, clearly due to the simulated tidal effects. It is worthwhile remarking here that both the periodic effect and the peaks

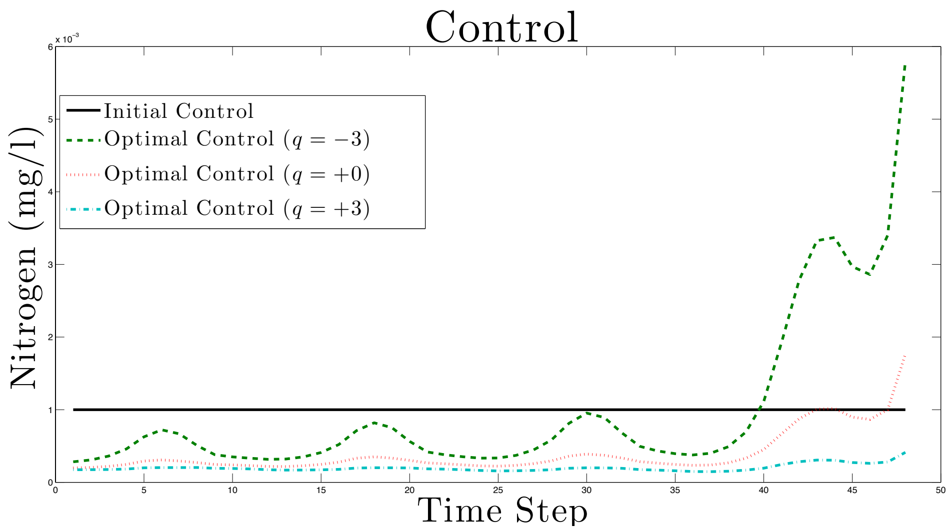

Figure 2: Uncontrolled nitrogen discharge, and optimal nitrogen discharges for the three wastewater locations under study ($q = -3$, $q = 0$, and $q = 3$).

reached at final time (due to the fact that the cost function only takes into account what happens in our time interval of about four tidal periods, dismissing later effects) have already been observed by the authors in previous related works.

Finally, we must also remark that in the three numerical test analyzed in this section, the state constraints related to nitrogen and phytoplankton concentrations are active, reaching the corresponding upper bounds at some instant.

6 CONCLUSIONS

In this paper we have shown the usefulness of a combination of optimal control theory and mathematical simulation in the resolution of environmental control problems. In particular, we have dealt with the limitation of eutrophication processes inside a sensitive zone by the control of the wastewater discharges in the region. In this case, the main difficulties are due to the fact that the problem is posed on a free-boundary moving domain, which prevents us from employing standard tools, leading us to the use of ALE techniques to deal with the non-cylindrical domain. In addition to a theoretical analysis of the problem (existence of optimal solutions, characterization of solutions by a first order optimality system), a complete numerical algorithm for its solving has been proposed (including the resolution of the hydrodynamical problem, the computation of the concentrations for the different species, and the numerical optimization of the fully discretized problem). Finally, all these skills have demonstrated their effectiveness in the resolution of a simplified problem under different scenarios, allowing a comparison of the optimal results.

ACKNOWLEDGEMENTS

The research contained in this work was supported by Project MTM2012-30842 from Ministerio de Economía y Competitividad (Spain) and FEDER.

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