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ALGAL CULTIVATION FOR BIOENERGY PRODUCTION: FIRST MATHEMATICAL MODELLING RESULTS IN RACEWAYS

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Summary. The most used algae cultivation systems are the open-channel raceway ponds for their low maintenance and energy costs. Raceways allow algal cultivation using wastewater, where algae mass can be employed as source for bioenergy production. One of the main external factors influencing algal productivity is the velocity of the liquid inside the pond, that can be easily controlled by the position and/or rotational speed of the turning paddle wheel, and by the height of water. In this work we introduce a novel methodology to automate the optimization of the design of raceway ponds based on techniques of optimal control of partial differential equations. So, we formulate the problem as a control problem where the state system is given by the coupled nonlinear equations for hydrodynamics and algae/nitrogen/phosphorus concentrations, and the objective function to be maximized represents the global concentration of algae at final time. We present here a detailed, rigorous mathematical formulation of the optimal control problem, we propose a numerical algorithm for its resolution, and we show some preliminary computational results related to the numerical modelling of the problem.

1 INTRODUCTION

Wastewater treatment by algae-based technologies is an effective solution that allows, as a by-product, the recovery of materials that can be used, for instance, to produce bioenergy (biodiesel, bioalcohol, etc.) due to the richness of lipides of the algal biomass coming from wastewater treatments.

The most used algae cultivation systems are the open-channel raceway ponds (open channels in the shape of an oval equipped with a rotating paddle wheel in order to promote the recirculation of the shallow water inside them) for their low maintenance and energy costs. Raceways allow algal cultivation using wastewater and, once the algae mass has grown enough, it is recovered by any mechanical/chemical harvesting method, and can be employed as source for bioenergy production [1, 2].

One of the main external factors influencing algal productivity is the velocity of the liquid inside the pond, that can be easily controlled by the position and rotational speed of the turning paddle wheel and also by the fixing of water height inside the raceway. The optimal design of raceway ponds has been widely studied within the scientific literature, but mainly by the comparison of case studies and the use of statistical techniques [3]. Nevertheless, the application of techniques of optimal control of partial differential equations -as it is our proposal- for the simultaneous optimization of speed and position of the rotating paddlewheel has remained completely unaddressed, as far as we know.

In this work we introduce a novel methodology to automate the optimization of location and management of the paddlewheel in a raceway pond. So, we formulate the problem as an optimal control problem where the state system is given by the coupled nonlinear equations for hydrodynamics and algae/nitrogen/phosphorus concentrations [4], the control variables are height of water and location and rotational speed of the paddlewheel, and the objective function to be maximized represents the global concentration of algae at final time.

In this paper we present a detailed, rigorous mathematical formulation of the control problem, we propose a numerical algorithm for its resolution and we show some preliminary computational results related to the numerical modelling of the problem.

Figure 1: Open-channel raceway ponds in California, U.S. (Source: www.atlanticgreenfuels.com)

2 MATHEMATICAL SETTING OF THE PROBLEM

In this section we introduce the mathematical formulation of the real-world problem, which is a necessary and decisive first step in order to its resolution. In the first part, we present the complex mathematical system modelling the main phenomena that appear in the physical problem. Then, we formulate the optimal design problem as a control-constrained optimal control problem.

2.1 Mathematical Model: The State System

We consider a moving liquid domain $\Omega(t) \subset \mathbb{R}^3$, for each t in a time interval $I = (0,T)$, representing the open raceway pond occupied by shallow waters, where $\Gamma(t)$ is the boundary of $\Omega(t)$. We consider the boundary $\Gamma(t)$ divided into two parts $\Gamma(t) = \Gamma_1(t) \cup \Gamma_2(t)$, where $\Gamma_1(t)$ corresponds to the bottom and the lateral walls, and $\Gamma_2(t)$ corresponds to the top free surface. Finally, we denote by $\vec{n}(t)$ the unit outward normal vector to the boundary $\Gamma(t)$.

For the sake of simplicity, we will assume that, at initial time $t = 0$, the pond presents a fixed constant height of water $H > 0$ (that is, $\Omega(0) = G \times [0,H]$, with $G \subset \mathbb{R}^2$ representing the ground plan of the raceway, as given in Fig. 2), where water is initially at rest.

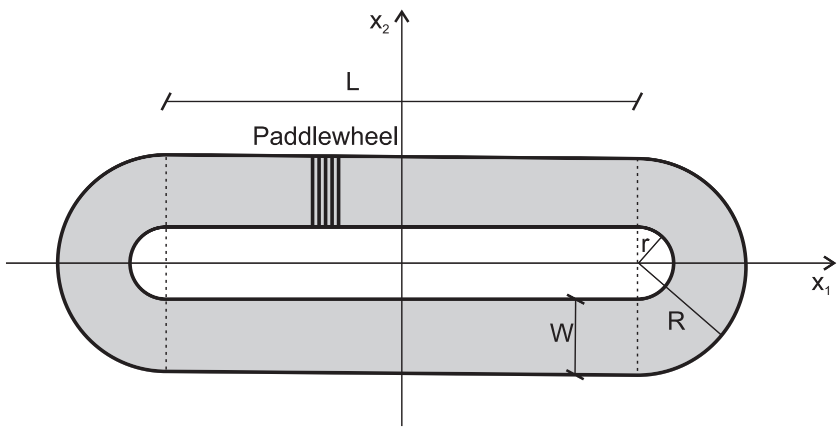

Figure 2: Schematic drawing of the raceway ground plan G, showing the two straight channels of length L and width W, and the two semicircular channels of radii r and R. A possible location for the paddlewheel is also shown.

Our state variables include velocity $v(x,t)$ and pressure $p(x,t)$ of the liquid at time $t \in I$ and at point $x = (x_1, x_2, x_3) \in \Omega(t)$, given by the classical Navier-Stokes equations for incompressible flows:

$$\begin{cases} \dfrac{\partial \vec{v}}{\partial t} + (\vec{v} \cdot \nabla)\vec{v} - \mu \Delta \vec{v} + \nabla p = \vec{F} \quad \text{in } \Omega(t),\ t \in I, \\ \nabla \cdot \vec{v} = 0 \quad \text{in } \Omega(t),\ t \in I, \\ \vec{v} = \vec{0} \quad \text{on } \Gamma_1(t),\ t \in I, \\ \vec{v}(x,0) = 0 \quad \text{in } \Omega(0), \end{cases} \tag{1}$$

where μ is the dynamic viscosity coefficient, and the second-member term $\vec{F}(x,t) = (F_1, F_2, F_3)$ represents the effect of the rotating paddlewheel with its axis centered at point (x_1^0, x_2^0, x_3^0) and with angular speed ω (see full details, for instance, in [5]), that is, for a force magnitude of F:

$$\begin{aligned} F_1(x,t) &= F\omega^2 \cos(\omega t)[(x_1 - x_1^0)^2 + (x_3 - x_3^0)^2], \\ F_2(x,t) &= 0, \\ F_3(x,t) &= F\omega^2 \sin(\omega t)[(x_1 - x_1^0)^2 + (x_3 - x_3^0)^2], \end{aligned} \tag{2}$$

in the water region $R(t)$ where the paddles rotate, and $\vec{F}$ null in the rest of the raceway. (A more detailed definition of region $R(t)$ will be given in bellow sections).

In addition to water state variables $v(x,t)$ and $p(x,t)$, we also consider the state variables corresponding to algal concentration $A(x,t)$, nitrogen concentration $N(x,t)$, and phosphorus concentration $P(x,t)$, given by the following coupled nonlinear system of convection-diffusion-reaction equations with Monod kinetics [4, 6], and with liquid velocity $\vec{v}$ obtained from previous state system (1):

$$\left\{ \begin{array}{l} \dfrac{\partial A}{\partial t} + \vec{v} \cdot \nabla A - \mu_A \Delta A = -\gamma A + L \, \dfrac{N}{K_N + N} \, \dfrac{P}{K_P + P} \, A \quad \text{in } \Omega(t), \ t \in I, \\ \dfrac{\partial N}{\partial t} + \vec{v} \cdot \nabla N - \mu_N \Delta N = -C_N L \, \dfrac{N}{K_N + N} \, A \quad \text{in } \Omega(t), \ t \in I, \\ \dfrac{\partial P}{\partial t} + \vec{v} \cdot \nabla P - \mu_P \Delta P = -C_P L \, \dfrac{P}{K_P + P} \, A \quad \text{in } \Omega(t), \ t \in I, \\ \dfrac{\partial A}{\partial n} = 0 \quad \text{on } \Gamma_1(t), \ t \in I, \\ \dfrac{\partial N}{\partial n} = 0 \quad \text{on } \Gamma_1(t), \ t \in I, \\ \dfrac{\partial P}{\partial n} = 0 \quad \text{on } \Gamma_1(t), \ t \in I, \\ A(x,0) = A_0(x) \quad \text{in } \Omega(0), \\ N(x,0) = N_0(x) \quad \text{in } \Omega(0), \\ P(x,0) = P_0(x) \quad \text{in } \Omega(0), \end{array} \right. \tag{3}$$

where the light rays effect L on algae is given by the expression:

$$L(x,t) = \mu_{max} \Theta^{\theta(t) - \theta_0} I(t) \, e^{-\Phi x_3}$$

with μ_{max} the maximum specific growth rate, Θ the thermic regeneration coefficient, $\theta(t)$ the temperature, θ_0 a reference temperature, $I(t)$ the incident light intensity, and Φ the coefficient for light attenuation due to depth. The other parameters in state system (3) are μ_A, μ_N and μ_P (corresponding to the diffusion coefficients of algae, nitrogen and phosphorus, respectively), γ (the algal death rate), K_N and K_P (the half-saturation constant for nitrogen and phosphorus, respectively), and C_N and C_P (representing the stoichiometric relations for nitrogen and phosphorus, respectively).

2.2 Optimal Design: The Optimal Control Problem

As above commented, in this study we are interested in finding the optimal initial height H of water, and the optimal location (x_1^0, x_2^0, x_3^0) and rotational speed ω of the paddlewheel, such that the production of algal biomass is maximized.

With respect to the water control variable H, this one must remain between a lower bound and an upper one, imposed by the geometric characteristics of the raceway.

With respect to the paddlewheel control variables, if we consider a wheel with paddles of length ρ, we will fix, for technical reasons, the coordinate x_3^0 as $\rho + \rho_0$, with ρ_0 small (so that the paddle does not pass too close to the bottom of the raceway). Moreover, due to the symmetry of the pond, we can restrict our study to only one of the two parallel straight channels -say the left one (see Fig. 2)- and we will fix the coordinate x_2^0 as the value corresponding to the central width of this left half of the raceway. So, in the end, we only have two paddlewheel control variables left, x_1^0 and ω, both subject to the appropriate geometric and/or technological constraints.

Since we are interested in optimizing the production of algae in the raceway, we are led to find the optimal values for H, x_1^0 and ω -all subject to their corresponding constraints- that maximize the cost functional:

$$J(H, x_1^0, \omega) = \int_{\Omega(T)} A(x, T)\, dx, \tag{4}$$

where the control variables H and (x_1^0, ω) enter the cost function via the definition of $\Omega(0)$ and the second member $\vec{F}$ of the system (1) corresponding to the state variable $\vec{v}$, respectively.

In the case that the state variable A is not regular enough (for instance, not continuous at $t = T$, but integrable) alternative cost functionals could be used instead, for instance:

$$J(H, x_1^0, \omega) = \int_0^T \int_{\Omega(t)} A(x, t)\, dx\, dt, \tag{5}$$

With respect to the regularity of the state variables, it is worthwhile recalling here that, as it is well known, the existence and regularity of the three-dimensional Navier-Stokes system (1) is still an open problem. However, if we assume that the velocity $\vec{v} \in [L^\infty(I; W^{1,\infty}(\Omega(t))]^3$, the authors have demonstrated in [4] that for smooth and bounded initial data, that is,

$$\begin{aligned} &A_0, N_0, P_0 \in L^2(\Omega(0)), \\ &0 \le A_0(x), N_0(x), P_0(x) \le M, \ \forall x \in \Omega(0), \end{aligned}$$

then the state variables A, N and P are also smooth and bounded. In particular, we have that:

$$\begin{aligned} &A, N, P \in W^{1,2,2}(I; H^1(\Omega(t)), H^1(\Omega(t))') \cap \mathcal{C}([0,T]; L^2(\Omega(t))), \\ &0 \le A(x,t), N(x,t), P(x,t) \le C(M,T), \ \forall x \in \Omega(t), \ t \in I, \end{aligned}$$

where the Bochner-Sobolev space $W^{1,2,2}(I; H^1(\Omega(t)), H^1(\Omega(t))')$ corresponds to the subspace [7]:

$$\{u \in L^2(I; H^1(\Omega(t))) \ / \ \frac{\partial u}{\partial t} \in L^2(I; H^1(\Omega(t))')\}.$$

3 NUMERICAL IMPLEMENTATION

For the numerical resolution of the state system of above optimal control problem (i.e., computing algal concentration for finding the optimal initial water height and the optimal paddlewheel location and rotational speed), the three-dimensional hydrodynamic model TELEMAC-3D [8] was used, where the WAQTEL biomass module was activated to include the effects of algal growth. Moreover, to treat the advective terms appearing in the state system, the option for the Multidimensional Upwind Residual Distribution (MURD) method was chosen.

Then, once we have computed a discrete approximation of the state variables (in particular, the discretized concentration of algae $A_h^n(\cdot) \simeq A(\cdot, t_n)$, for the set of discrete times t_n, $n = 0, 1, \ldots, N$), in order to calculate a discrete approximation J_h of the cost functional J given by (4), we can use any standard quadrature rule for the numerical integration over the spatial domain.

In this way, we will arrive to a discrete, constrained maximization problem, whose solution can be obtained by any numerical optimization algorithm, in particular, and for the sake of simplicity, by any derivative-free algorithm. In the present case we will propose, for instance, the Nelder-Mead method [9], after the inclusion of a suitable penalty term to deal with the bound constraints of the control variables.

3.1 Some numerical examples

This subsection presents only one of the many computational tests performed for the mathematical modelling of a real-world scenario posed in a raceway whose dimensions (measured in meters) are: length of straight channels $L = 20.0$, width $W = 2.0$, and radii $r = 0.2$ and $R = 2.2$. As above commented, the numerical experiences presented here have been developed with the open-source hydrodynamics module TELEMAC-3D, although in order to compare our results we have also tried the commercial program MIKE21 and the open software FreeFem++.

In the numerical simulation presented here, for the paddlewheel we have chosen the following data: paddle length $\rho = 0.4$, $\rho_0 = 0.1$ (and consequently $x_3^0 = 0.5$), and force magnitude $F = 10.0$. According to the geometry of the domain, location and angular speed have been taken as $x_1^0 = -5.0$ and $\omega = 0.5$, respectively. Finally, the water height has been taken as $H = 0.3$.

Taking into account previous considerations and data, in this case the region of influence of the paddles for the force term $\vec{F}$ in (1) is given by the following horizontal cylindrical segment:

$$R(t) = \{(x_1, x_2, x_3) \in \Omega(t) \ / \ 0.2 \leq x_2 \leq 2.2,\ (x_1 - x_1^0)^2 + (x_3 - x_3^0)^2 \leq \rho^2\},$$

i.e., for suitable coordinates (x_2, x_3), coordinate x_1 varies between $x_1^0 - \sqrt{\rho^2 - (x_3 - x_3^0)^2}$ and $x_1^0 + \sqrt{\rho^2 - (x_3 - x_3^0)^2}$. We must remark here that the region of influence of the paddles is independent of angular speed ω, depending only on location x_1^0 and height H.

With respect to other data for the state systems, for a time t measured in seconds, temperature θ (measured in °C) is given by:

$$\theta(t) = 20 + 2\sin\left(\frac{2\pi t}{86400}\right),$$

(that is, oscillating between 18 and 22 along the whole day), considering a reference temperature of $\theta_0 = 20$. Finally, incident light intensity I is given by expression:

$$I(t) = \max\left\{0, \sin\left(\frac{2\pi t}{86400}\right)\right\}$$

which means that is null overnight.

For the sake of conciseness, we will present here only one numerical test from the many developed by the authors. So, in Fig. 3 we show an example of the numerical results corresponding to the field of water velocities for the final time $T = 86400$ seconds (corresponding to one day).

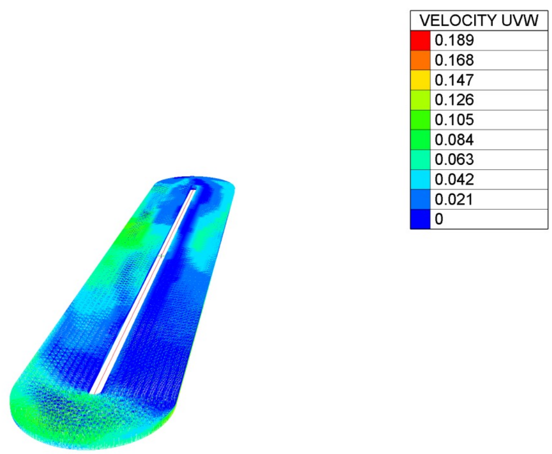

Figure 3: Computational water velocities obtained for the raceway mesh at final time.

All the numerical results obtained in the numerous computational tests developed for the modelling step in the resolution of the optimal control problem have shown a good performance. So, we are now focused on the optimization step for the resolution of the optimal control problem, whose numerical results will be presented in a forthcoming paper.

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