

A COMPUTATIONAL FRAMEWORK FOR INFORMING DECISION IN RELATION TO ENVIRONMENTAL IMPACT OF WASTEWATER DISCHARGES

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Abstract. Multi-objective optimization combined with numerical simulation are useful tools for environmental sciences. Using these methods, the treatment and discharge of wastewater in large waterbodies (estuaries, rivers, lakes. . .) - one of the essential problems in environmental management - can be analyzed in order to avoid the usual controversy between economic and ecological interests. In this article we present a decision support software system referred to as *Simulating Optimal Solutions* (SOS). Software SOS is a Matlab toolbox (interfaced with Fortran codes for mathematical computation of hydrodynamics and contaminant dispersion) to assess in decision making related to treatment intensity in different purifying plants. The program allows a flexible analysis both from a cooperative viewpoint (Pareto optimality) and a non-cooperative one (Nash equilibria). A realistic example posed in Arousa estuary (NW Spain) helps us to show its capabilities.

1 Introduction

Waste elimination is one of the most important environmental problems nowadays. For the particular case of wastewater in urban areas, domestic sewage and trade waste are collected from different districts and transported to purifying plants *via* pipes and

pumping stations. These plants treat sewage by different biochemical methods and, finally, treated effluents are discharged through subsurface outfalls into aquatic media (a lake, a river, an estuary...). Sewage treatment is not only a necessary task but also a very expensive one, and determining the intensity of the treatment has become a very difficult problem involving both environmental and economic aspects.

Mathematical modelling can be already considered as a classical tool in the field of environmental water management (specially related to river, estuarine and coastal waters) and there is a great number of computational works (along with commercial software) to simulate coastal or river hydrodynamics and pollutant transport. In last few decades, the utility of optimization and control techniques for this type of problems has been made clear in several works. More recently, the authors [4, 1, 2] have combined optimal control theory with multi-objective optimization techniques to determine efficient discharge strategies in the management of a wastewater treatment system.

The main aim of this paper is introducing SOS (acronym for *Simulating Optimal Solutions*), a numerical simulation toolbox (based on the theory developed by the authors in previous works) to help in decision making related with the intensity of the purification in a wastewater treatment system. The paper is organized as follows: In Section 2 we present the problem and briefly recall the mathematical models and the approximation techniques employed in the numerical simulation. In Section 3 we formulate, for different possible scenarios, the problem of determining the intensity of the treatment in a system of purifying plants, and introduce several concepts of optimal solutions. The organization of software SOS is presented in Section 4, and its usage is exemplified with a realistic problem in Section 5. Finally, some conclusions are summarized in Section 6.

2 Mathematical models and numerical simulation

First of all we introduce the environmental problem: We consider an urban area with a wastewater treatment system consisting of N_E purifying plants, which collect sewage from different districts, treat it with different methods and, finally, discharge the treated effluents into a shallow water domain Ω (for example, an estuary) through submarine outfalls located at points $b_j \in \Omega$, $j = 1, \dots, N_E$ (see a scheme in Fig. 1).

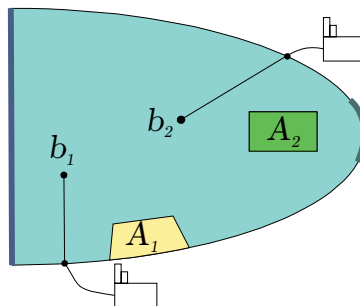


Figure 1: Scheme of domain Ω

Moreover, we assume the existence of several sensitive areas $A_i \subset \Omega$, $i = 1, \dots, N_Z$ (representing fisheries, beaches or marine recreation zones), where the water quality should be guaranteed with pollution levels lower than some allowed thresholds (fixed by administrative directives). The problem consists of determining the intensity of the treatment in each plant during an arbitrary period of time $(0, T)$. The strategy should satisfy two objectives: (a) it should be *cheap* (low economic cost), and (b) it should be *green* (low environmental impact); but because these objectives are opposite there will not be a unique best strategy. In next section, we will introduce the concepts of optimal solutions for the problem in two different possible situations (each plant is controlled by a different organization, a unique organization controls all plants), but previously we need to deal with the numerical simulation of the environmental impact caused by pointwise wastewater discharges in a shallow water domain.

For the numerical simulation we take into account that the flow of an effluent from a submarine outfall in a shallow water domain is mainly governed by horizontal transport due to currents (produced by wind, tide and so on) and turbulent diffusion. This fact allows us to uncouple hydrodynamical system (shallow water equations) from transport system (advection-diffusion-reaction equations): The former gives the height of the water column and the velocity field which are used in the latter to obtain the pollution levels.

2.1 Hydrodynamic model: The shallow water equations

If we consider Γ , the boundary of Ω , divided into three different parts $\Gamma = \Gamma^- \cup \Gamma^+ \cup \Gamma^0$ (as can be seen in Fig. 1), with Γ^- corresponding to inflow, Γ^+ corresponding to open sea, and Γ^0 corresponding to the coast, then the shallow water (SW) equations can be written as:

$$\left. \begin{aligned} \frac{\partial h}{\partial t} + \vec{\nabla} \cdot (h\vec{u}) &= 0, & \frac{\partial \vec{u}}{\partial t} + (\vec{u} \cdot \vec{\nabla})\vec{u} - \nu \Delta \vec{u} + g\vec{\nabla}h &= \vec{F} & \text{in } \Omega \times (0, T), \\ h = \eta, \quad \vec{u} \cdot \vec{n} &= q & & & \text{on } \Gamma^- \times (0, T), \\ h = \phi, \quad \vec{\nabla} \cdot \vec{u} &= 0 & & & \text{on } \Gamma^+ \times (0, T), \\ \vec{u} \cdot \vec{n} &= 0 & & & \text{on } \Gamma^0 \times (0, T), \\ h(0) = h_0, \quad \vec{u}(0) &= \vec{u}_0 & & & \text{in } \Omega, \end{aligned} \right\} \quad (1)$$

where $h(x, t)$ and $\vec{u}(x, t)$ denote, respectively, the height of water and the depth-averaged horizontal velocity of water, initial and boundary data $\eta(x, t)$, $\phi(x, t)$, $h_0(x)$, $q(x, t)$ and $\vec{u}_0(x)$ are given functions, ν (kinetic eddy viscosity coefficient) and g (gravity acceleration) are physical parameters experimentally known, \vec{n} denotes the unit outer normal vector to boundary Γ , and the source term $\vec{F}(x, t)$ collects all the effects of atmospheric pressure, wind stress, bottom friction and so on.

System (1) can be solved by finite difference, finite element or finite volume methods. Software SOS includes a Fortran code (`Shallow-Water.exe`) based in classical results [3], which has been successfully applied by the authors in several previous works.

2.2 Pollutant dispersion: The faecal coliform model

Since we are considering domestic discharges, we will take *faecal coliform* (FC) concentration as a water quality indicator. The FC concentration in a shallow water domain is given by equation:

$$\left. \begin{aligned} \frac{\partial \rho}{\partial t} + \vec{u} \cdot \vec{\nabla} \rho - \beta \Delta \rho + \kappa \rho &= \frac{1}{h} \sum_{j=1}^{N_E} m_j(t) \delta(x - b_j) && \text{in } \Omega \times (0, T), \\ \frac{\partial \rho}{\partial n} &= 0 && \text{on } \Gamma \times (0, T), \\ \rho(0) &= \rho_0 && \text{in } \Omega, \end{aligned} \right\} \quad (2)$$

where $\rho(x, t)$ is the depth-averaged FC concentration, $h(x, t)$ and $\vec{u}(x, t)$ are the solution of the shallow water system (1), $\beta > 0$ is a given viscosity coefficient collecting turbulent and dispersion effects, $\kappa \geq 0$ is an experimental coefficient related to the loss rate of FC, $m_j(t)$ is the mass flow rate of FC discharged through the outfall located at point b_j , $\delta(x - b_j)$ denotes the Dirac measure centered at b_j , and $\rho_0(x)$ represents the initial datum.

Software SOS includes a new Fortran code (`Faecal-Coliform.exe`) - also developed by the authors - based on a finite element discretization with good convergence properties, in order to solve equation (2).

3 Mathematical formulation

As above mentioned, our main aim consists of determining the treatment intensity on each one of the purifying plants of the system. The first step in order to formulate the problem in a correct way relies in fixing the exact targets to reach. Although these objectives are basically of two types, economic and ecological, there exist many external circumstances that can modify the precise definition of each one of them. Related to this, we will state two different situations: A first case where each plant is managed by a different organization (scenario I), and a second case where there exists a unique organization controlling the whole depuration system (scenario II).

3.1 Scenario I

First, we will assume that each one of the plants is controlled by a different organization (for example, diverse municipal governments) and we will impose that each organization has to take care of a small number of sensitive areas, in such a way that a penalty is imposed on the plant if the water pollution levels in some of its associated zones is greater than a fixed threshold level. As it is obvious, in this case, there exist as many objective functions as purifying plants, that is, there are N_E cost functions. Moreover, determining the intensity of the treatment in each purification plant is equivalent to determining the amount of FC discharged after purification; consequently, each plant manages one control (or design variable) in equation (2): the function $m_j(t)$ will be the control associated to

the j -th plant, in a set of feasible controls $M_j \subset L^\infty(0, T)$, where $L^\infty(0, T)$ denotes the space of bounded functions in $(0, T)$.

The cost function for the j -th plant collects two different aspects: (a) the *purification process cost*, and (b) the *cost because of insufficient purification* (penalties). The purification process cost in a plant is related to FC discharge through the corresponding outfall and, for the interval time $(0, T)$, it will be given by $\int_0^T f_j(m_j(t)) dt$, where f_j is a known function which depends on the characteristics of plant. About penalties, the j -th plant has to take care of some sensitive areas $(A_1^j, \dots, A_{n_j}^j)$ and, if purification is insufficient and the FC concentration in A_i^j is greater than a fixed threshold σ_i^j (which depends on the type of area), a penalty will be imposed. We also assume that penalty amount is an increasing (quadratic) function of FC concentration surpassing the desired threshold. Thus, for the time interval $(0, T)$, the total penalty will be given by expression $\sum_{i=1}^{n_j} \frac{1}{2\epsilon_i^j} \int_0^T \int_{A_i^j} (\rho(x, t) - \sigma_i^j)_+^2 dx dt$, where ϵ_i^j is a given penalty parameter, also depending on the type of area.

Then, in this case, the problem of determining the intensity of the treatment in each plant of the depuration system can be formulated as the following multi-objective problem:

PROBLEM 1: Find $m(t) = (m_1(t), \dots, m_{N_E}(t)) \in M = \prod_{j=1}^{N_E} M_j$ which minimizes the cost functionals

$$J_j(m) = \int_0^T f_j(m_j(t)) dt + \sum_{i=1}^{n_j} \frac{1}{2\epsilon_i^j} \int_0^T \int_{A_i^j} (\rho(x, t) - \sigma_i^j)_+^2 dx dt, \quad (3)$$

for $j = 1, \dots, N_E$, and where $\rho(x, t)$ is the solution of the state equation (2).

It is clear that, due to the contradictory character of these cost functions, there will not exist a *utopic* (or ideal) solution $m = (m_1, \dots, m_{N_E}) \in M$ minimizing simultaneously all the cost functionals J_j , $j = 1, \dots, N_E$. Then, we are led to seek a more realistic type of optimal solution. In this spirit, software SOS can compute cooperative (Pareto-optimal) and non-cooperative (Nash equilibria) solutions for Problem 1.

3.1.1 Non-cooperative solutions: A Nash equilibrium

If each plant manager looks for its own purification strategy (that is, its own control m_j) in order to minimize its own cost functional J_j , software SOS gives a whole strategy (a vector of controls $m = (m_1, \dots, m_{N_E})$) which should be accepted by all of the plant managers. This whole strategy is such that none can change its particular strategy without increasing its particular cost functional, if the others do not change their respective strategies. In game theory, this vector $m \in M$ is known as a Nash equilibrium. To be exact, $m = (m_1, \dots, m_{N_E}) \in M$ is a Nash equilibrium if it verifies that, for all $j = 1, \dots, N_E$,

$$J_j(m_1, \dots, m_{j-1}, m_j, m_{j+1}, \dots, m_{N_E}) = \min_{m_j^* \in M_j} J_j(m_1, \dots, m_{j-1}, m_j^*, m_{j+1}, \dots, m_{N_E}), \quad (4)$$

where M_j represents the set of feasible controls for the j -th plant.

Software SOS computes a Nash equilibrium m for Problem 1 by solving the necessary optimality system:

$$\frac{\partial J_j}{\partial m_j}(m) = 0, \quad j = 1, \dots, N_E. \quad (5)$$

In order to do this, the program uses a standard method for solving nonlinear systems, where partial derivatives in (5) are computed from the *sensibilities* with a Fortran code (`Sensibility.exe`) whose details can be seen in the technical paper [5].

3.1.2 Cooperative solutions: A Pareto-optimal frontier

However, if plant managers are ready to cooperate, a Nash equilibrium can be not an optimal solution because a *better* vector of controls can exist, bringing off a simultaneous decrease of all cost functions. In a cooperative situation, an optimal solution is a vector of controls $m = (m_1, \dots, m_{N_E}) \in M$ where none of the components can be improved without deterioration of, at least, one of the other components. These vectors are usually called Pareto-optimal solutions. A more formal definition can be given: $m = (m_1, \dots, m_{N_E}) \in M$ is a Pareto-optimal solution if there does not exist any $m^* \in M$ such that $J_j(m^*) \leq J_j(m)$, for all $j = 1, \dots, N_E$, and such that, for at least one $j \in \{1, \dots, N_E\}$, $J_j(m^*) < J_j(m)$. If $m \in M$ is a Pareto-optimal solution, the objective vector $(J_1(m), \dots, J_{N_E}(m)) \in \mathbb{R}^{N_E}$ is also known as Pareto-optimal. The set of Pareto-optimal solutions is called the Pareto-optimal set, and the set of Pareto-optimal objective vectors is called the Pareto-optimal frontier.

Software SOS can represent in a graphic the Pareto-optimal frontier (and the corresponding Pareto-optimal solutions) for Problem 1, by using the classical weighting method as described in [1]. Objective functions J_j and their gradients are again evaluated from the *sensibilities* (see [5]).

3.2 Scenario II

In the case that there exists a unique organization (for instance, a central government) managing all the plants of the deputation system, the objectives need to be redefined. The purification process cost can be treated in a global way (as an unified objective), but the penalties for insufficient deputation should be divided by zones (as many objectives as sensitive areas), because in this manner it can be possible the detection, for a same cost, of several deputation options that will favour (from a ecological viewpoint) one area over another. Among the different optimal options, will be the decision maker who (invoking possible ecological, commercial or political criteria) will select one of them.

In this situation, the problem can be formulated in the following way:

PROBLEM 2: Find $m(t) = (m_1(t), \dots, m_{N_E}(t)) \in M$ which minimizes the cost functionals:

$$K_C(m) = \sum_{j=1}^{N_E} \int_0^T f_j(m_j(t)) dt, \quad (6)$$

$$K_i(m) = \frac{1}{2\epsilon_i} \int_0^T \int_{A_i} (\rho(x, t) - \sigma_i)_+^2 dx dt, \quad \text{for } i = 1, \dots, N_Z, \quad (7)$$

and where $\rho(x, t)$ is the solution of the state equation (2).

By using similar techniques to those applied for solving previous Problem 1, software SOS computes the Pareto-optimal frontier and the corresponding Pareto-optimal solutions for Problem 2 (non-cooperative solutions do not make any sense in this case).

4 Software organization

Software SOS is a compiled Matlab code which is presented with an installer program including the Matlab libraries *MCR Compiler*. In this way, the software SOS can be installed and run in any computer under Windows operative system, even in the case that Matlab program has not been installed on it. Software SOS is organized in three different modules: *Hydrodynamics*, *Management* and *Pollution*. The central core of each module is formed by a Fortran routine solving the system of partial differential equations used in the resolution of the corresponding problem. These three modules, in spite of being completely independent, are interconnected one to another, in such a way that the output produced by one module can be used as input to another one. In Fig. 2 we present a simplified diagram showing the flow chart, where we can observe the relationships among the three modules (Mandatory inputs/outputs are represented by continuous lines, and optional inputs/outputs are represented by dashed ones). The complete task developed by each module is specified below:

- *Hydrodynamics*: This first module is devoted to the simulation of hydrodynamics in a domain occupied by shallow water. From the geometry of the domain and specific data of the hydrodynamic model, a Fortran code (**Shallow-Water.exe**) solves the SW system (1) obtaining, for a previously selected period of time, the height of the water column and the depth-averaged velocity of water in the whole domain.
- *Management*: This second module deals with the problem of the optimal management for a wastewater depuration system, in the terms above detailed in Section 3. Then, from given water height and velocity fields, and from previously selected out-fall locations and sensitive areas, a Fortran code (**Sensibility.exe**) determines all the data necessary in order to evaluate the objective functions and their derivatives. Once obtained these data, and using a suitable Matlab code, the module solves the problem previously selected by the user (Problem 1 in any of its possible formulations (cooperative and non-cooperative) or Problem 2), showing the optimal depuration strategies in each treatment plant of the system.

- *Pollution*: This third module simulates the evolution of FC concentration in the domain under study, starting from the height and velocity of water, and the location and intensity of wastewater discharges (which can be directly supplied by the user or provided by previous module *Management*). To do this, the system (2) is solved by a new Fortran code (*Faecal-Coliform.exe*), and the results are shown.

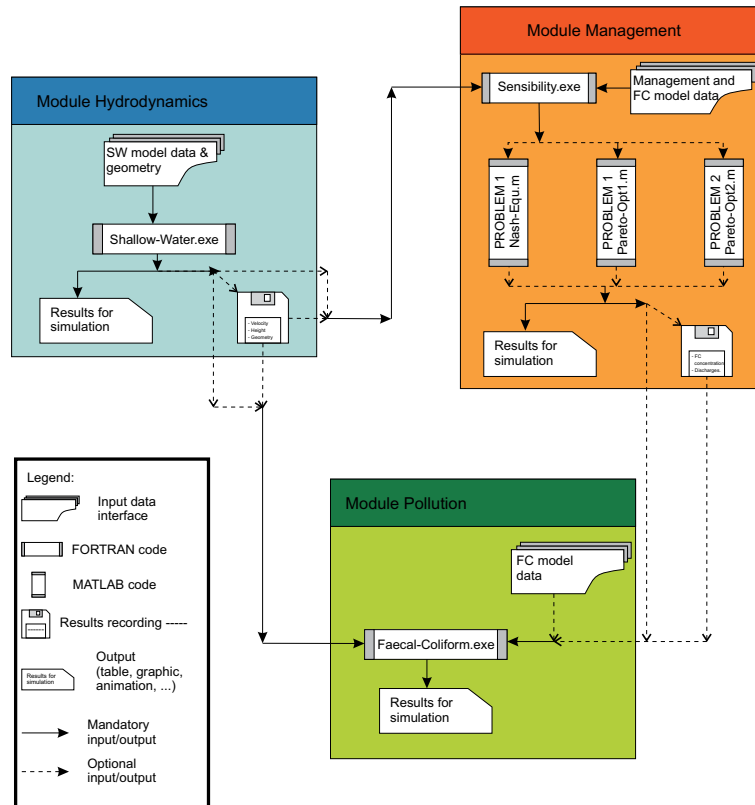


Figure 2: Diagram of SOS organization

5 Software demonstration: an illustrative example

In this section we exemplify the use of toolbox SOS by a realistic application posed in Arousa estuary, one of the more interesting zones - both from tourism and ecology viewpoints - in NW Spanish Atlantic coastline. As above commented, software SOS is composed of three main modules, that can be launched by the user from SOS initial interface (as shown in Fig. 3). These modules require several input parameters, and produce several output arguments (in some cases, the output in one module is the input for another one). Moreover, the toolbox gives the possibility of data recording in disc for later visualization and/or usage. In the next we explain the detailed whole process.



Figure 3: SOS initial interface

5.1 Hydrodynamics

When selecting “Hydrodynamics” in the SOS initial interface, a new interface (shown in Fig. 4) is opened. We must recall that the main goal of this module consists of solving the SW equations. Consequently, several input data are required for running the Fortran code `Shallow-Water.exe`. Thus, we charge a file containing the mesh for Arousa estuary, and specify the values for necessary parameters (water density, Chezy coefficient, wind velocity, (North) latitude, Bermúdez-Moreno parameter $\text{Rho} \in (0, 1)$, and so on) by means of several buttons and editable fields. Once completed the data input, the toolbox proceeds to compute the numerical solution of the system, making available to the user an output file (`*.mat`) with the hydrodynamic variables: water height $h(x, t)$ and velocity $\vec{u}(x, t)$, that SOS can also show in a graphic manner (either by an animation or by frames), as can be seen in Fig. 4.

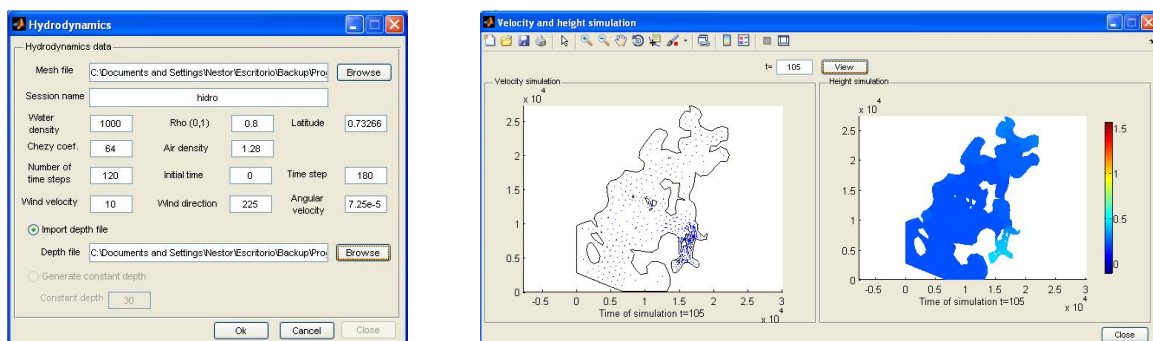


Figure 4: Hydrodynamics module interface (left), and an example of Hydrodynamics results (right)

5.2 Management

We continue with SOS performance by running the module *Management*, whose initial interface can be seen in Fig. 6. In order to run this module, it is necessary to import a previous session of the module *Hydrodynamics* (that is, the corresponding **.mat* file). Moreover, the outfall locations and the sensitive areas have to be given by the user in an interactive way (with the help of the mouse device). An example of this specifications is shown in Fig. 5.

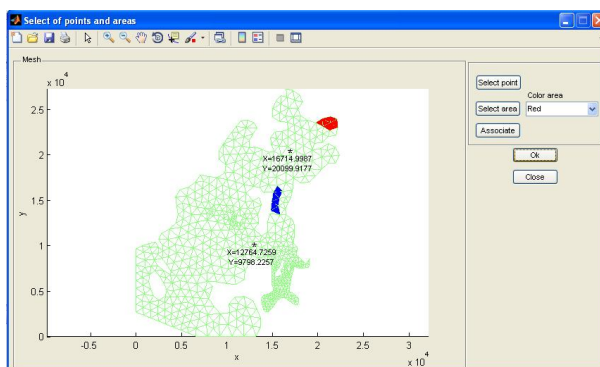


Figure 5: An example of selection (making use of the pointer) of outfall locations and sensitive areas

Next, the user must also provide SOS with the several physical parameters required for running the Fortran code *Sensibility.exe* (such as viscosity or loss rate of FC), with the data for FC model (initial discharges and maximal thresholds for FC concentrations in each area), and also with the parameters related to the numerical resolution (tolerance, maximum number of iterations, etc.)

Finally, the user has to select the exact type of problem to solve. In our particular case, we have chosen to solve Problem 1 *via* the computation of a Nash equilibrium with the Matlab code *Nash-Equ.m*, whose optimal (non-cooperative) strategy is shown in Fig. 6. In this figure we can see, in addition to a graphic output corresponding to the optimal discharges, a table presenting the problem data and also the final treatment costs (purification process cost CS , penalties PN , and total cost J). Again, software SOS gives us the possibility to save in disc our results, among others, the resulting discharges corresponding to the optimal treatment intensities.

5.3 Pollution

With the final objective of determining the ecological impact on Arousa estuary of a particular purification strategy, we launch the module *Pollution* by selecting “Pollution” in the SOS initial interface. After this, we need to import the previous sessions of *Hydrodynamics* and *Management* (by their corresponding **.mat* files), and then run the module. An example of the results obtained by this module are shown in Fig. 7. It is worthwhile

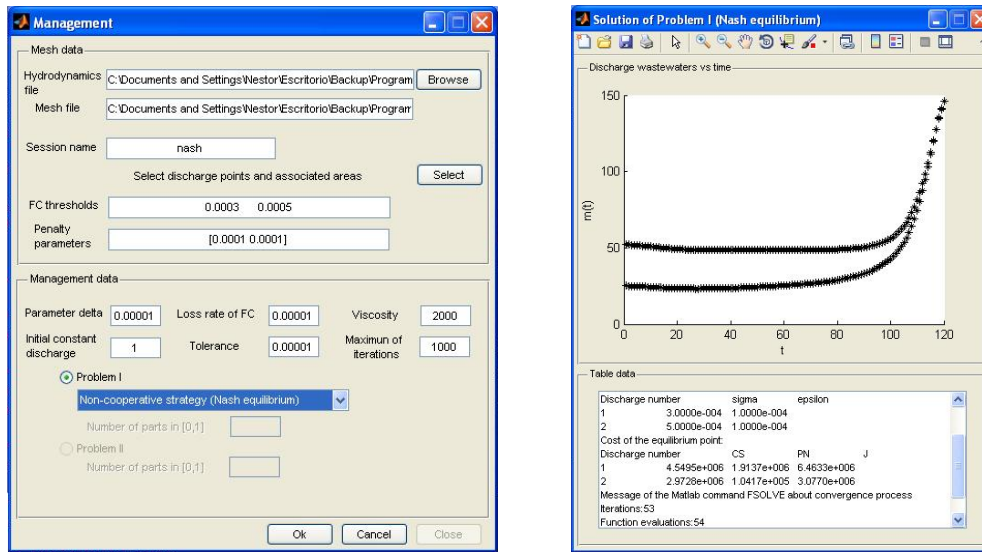


Figure 6: Two examples of interfaces for the Management module: input interface (left), and output interface (right)

remarking here that software SOS allows also to simulate the ecological impact of any discharge (not only an output of previous module *Management*) by the manual introduction from the user of necessary data (such as discharge intensities, outfall locations, etc.).

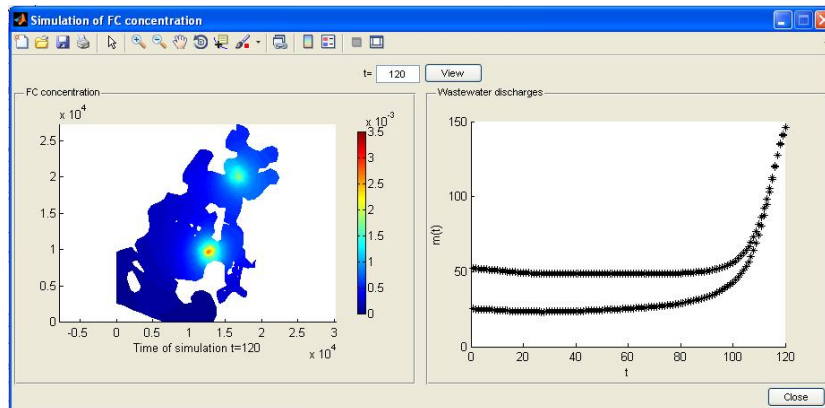


Figure 7: An example of Pollution results

6 Conclusions

This paper has presented new computer software to assess decision makers in questions related to wastewater treatment intensities in a depuration plant system. The Matlab toolbox SOS (from *Simulating Optimal Solutions*) is organized into three main modules originally designed to reach jointly this goal (although SOS also allows the individual

use of any of them). These three modules are *Hydrodynamics*, *Management* and *Pollution*. It is worthwhile remarking here that running first and third modules implies the numerical solution of a subordinate mathematical model (so, in *Hydrodynamics* we need to solve the SW equations (1), and in *Pollution* we solve the FC model (2)), and, in order to do this, software SOS incorporates its own Fortran codes (**Shallow-Water.exe** and **Faecal-Coliform.exe**, respectively). Moreover, for determining wastewater treatment intensities, software SOS presents the module *Management*, where, once fixed the parameters for economic and ecological costs derived from wastewater treatment, the user can formulate two possible multi-objective optimization problems: Problem 1 (each plant of the system controlled by a different organization) and Problem 2 (a unique organization controls the whole system). For the resolution of these problems, software SOS constructs its own cost functional, considers possible strategies (non-cooperative Nash equilibria or cooperative Pareto-optimal solutions) and incorporates accurate numerical methods based on the computation of the gradients (using the Fortran code **Sensibility.exe**) of the cost functionals. Finally, we must mention here that all above commented capabilities are developed on a intuitive and user friendly programming environment (as can be stated in the illustrative example) which is freely available for research purposes.

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REFERENCES

- [1] L.J. Alvarez-Vázquez, N. García-Chan, A. Martínez, M.E. Vázquez-Méndez, Multi-objective Pareto-optimal control: An application to wastewater management, *Comput. Optim. Appl.* 46 (2010) 135-157.
- [2] L.J. Alvarez-Vázquez, N. García-Chan, A. Martínez, M.E. Vázquez-Méndez, Pareto-optimal solutions for a wastewater treatment problem, *J. Comput. Appl. Math.* 234 (2010) 2193-2201.
- [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) 79-97.
- [4] N. García-Chan, R. Muñoz-Sola, M.E. Vázquez-Méndez, Nash equilibrium for a multiobjective control problem related to wastewater management, *ESAIM: Control Optim. Calc. Var.* 15 (2009) 117-138.
- [5] M.E. Vázquez-Méndez, L.J. Alvarez-Vázquez, N. García-Chan, A. Martínez, Improving the environmental impact of wastewater discharges with a specific simulation-optimization software, *J. Comput. Appl. Math.* 246 (2013) 320-328.