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Optimization of the spatial distribution of pollution emission in water bodies

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Contents

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Introduction

The environmental protection of water bodies in Europe is based on the Water Framework Directive, which combines the so called Emission Limits Value and the Water Quality Objective (QO) approaches. The first one sets limits to particular type of emissions, for example the Nitrate Directive, while the second establishes Quality Standards for Biological, Chemical and Hydromorphological Quality Elements, in order to ensure the functioning of freshwater and marine ecosystem and the sustainable use of water bodies. To this regard, mathematical models are valuable tools for reconciliating these approaches , since they allow one to establish a causal link between emission levels and the Quality Standards (”direct problem”) and viceversa (”inverse problem”).

In general, Quality Elements are variables or proper combination of variables which define the ”status” of a water body. For example, the ”chemical status” can be defined by a set of concentrations of chemicals which are potentially harmful for the ecosystem and humans, or the biological status may be based on Quality Elements which include the density of phytoplankton, the presence/absence of Submerged Aquatic Vegetation, the presence/absence of sensitive species etc. In many instances, the Quality Standards can then be expressed as threshold values, below or above which the functioning of the ecosystem is compromised and/or the risk for human health is not acceptable. If this is the case, management policies should be aimed at improving the state of the system and meet those Standards in the near future. In order to be carried in a cost-effective manner, such interventions should be based on a quantitative understanding of the relationships between the Pressures on the system and its State. This task could be very complex in large water bodies, where transport processes play a major role in creating marked gradients and pollution sources may be spatially distributed and/or not well identified. From the scientific point of view, the problem can be stated as follows: a mathematical model should enable one to "map" the spatial distribution of inputs (emissions) into the spatial distribution of the requested output, namely the "indicator" or "metric", which is subjected to a given constraint, the Quality Standard (QS), within the computational dominion. Such analysis may reveal that the QS are not respected only in a given fraction of the water body and, in the most favorable circumstances, identify the pollution sources which cause the problem. In such a case, a selective intervention, aimed at lowering the emission levels of those sources, would probably be more cost effective than the general reduction of the emission levels in the whole area. The spatial distribution of emission sources may also affect the pollution level and, in some instances, a proper redistribution of those sources in a given area, which leaves unchanged the total load, could have positive effect on the pollution level.

In this paper, we are going to investigate the above problems in the simplest possible setting, in order to provide a clear interpretation of the results in relation to the most relevant parameters. The paper is organized as follows: in the "methods" section, we present the basic equations and provide insights for solving the problem in the general case as well as in the specific one here presented. The analytical solutions are presented and discussed in the next two sessions and some concluding remarks are then summarized in the conclusive section.

Methods

In order to solve the problem analytically, we selected a 1D setting, which may be representative of a river or of a coastal area where the main current runs parallel to the coast line, and assumed that a given pollutant is discharged within a prescribed area, which, in this setting, is represented by an interval $[a, b]$ of length $L = b - a$. Furthermore, we assumed that:

i) the discharge rate does not depend on time;

ii) the dispersion of the pollutant is described by both advection and diffusion, but the water velocity and eddy diffusivity are both constant in space and time and

iii) the pollutant is removed from the water column by physico-chemical, chemical or biochemical processes, whose rate is proportional to its concentration.

Under the above restrictive hypothesis, the dynamic of the compound, u, is governed by the following PDE equation:

$$\frac{\partial u}{\partial t} + v\frac{\partial u}{\partial x} = \alpha\frac{\partial^2 u}{\partial x} - \lambda u + \rho(x). \tag{1}$$

in which:

– t is the time;

– x is the state variable;

– v is the constant water velocity;

– λ is a coefficient characterizing a decay rate of the pollutant and

– α is the eddy diffusion coefficient;

and $\rho(x)$ represent the discharge rate "density", i.e. the amount of pollutant which enter the water body per unit of time and space: due to our hypothesis, $\rho(x) = 0$ outside the interval $[a, b]$. Once ρ is specified, the total amount of pollutant discharged per unit of time, or *Total Load* (=TL), is given by the integral

$$\int_a^b \rho(x)dx \tag{2}$$

For example, equation (1) may represent the dynamic of a dissolved or suspended constituent, such as BOD, which decays according to first-order reaction rate or is removed by sedimentation.

Under the restrictions specified above, the solutions of the parabolic equation (1) converge to a steady state solution, which satisfies the equation:

$$v\frac{du}{dx} = \alpha\frac{d^2u}{dx^2} - \lambda u + \rho(x) \tag{3}$$

Equation (3) is the starting point of our analysis. Let us assume that the concentration of the pollutant should not exceed a given QS, u_0, anywhere in the spatial domain and, on the other end, that, due to limit to the emission, the discharge rate density could not exceed a given value ρ_0. We then may ask the following question: which distribution ρ guarantees the respect of the QS in a given river stretch or in a given portion of the coastal area, and, at the same time, allow to discharge the maximum total loads? In mathematical terms, we need to find the distribution that maximizes total load (2) under the constraints

$$0 \le \rho(x) \le \rho_0, \quad x \in [a, b] \tag{4}$$

on the discharge rate density and

$$0 \le u(x) \le u_0, \quad x \in R, \tag{5}$$

$$u(\pm\infty) = 0, \tag{6}$$

on the respective solution of the equation (3)

In order to simplify forthcoming analytic solution, we introduce new dimensionless variables

$$\tilde{x} = (x - a)/L, \qquad \tilde{u} = u/u_0, \tag{7}$$

that is on the phase space we shift the origin to the beginning of the interval of pollutant discharging and the length L takes as the unit, and in the space of solution the constraint level u_0 we also take as the unit. These changes lead equation (3) to the form ("tilde" in the notations is omitted):

$$vL\frac{\partial u}{\partial x} = \alpha\frac{\partial^2 u}{\partial x^2} - \lambda L^2 u + \rho(x)L^2/u_0.$$

Assuming that $v > 0$ and dividing the last equation by vL we get the equation:

$$A\frac{d^2u}{dx^2} - \frac{du}{dx} - \Lambda u = -R(x), \tag{8}$$

where

$$A = \alpha/(vL), \qquad \Lambda = \lambda L/v, \qquad R = \rho L/(u_0 v) \tag{9}$$

In the set of new variables, the total load is:

$$TL = u_0 v/L \int\limits_0^1 R(x)dx \to \max \tag{10}$$

Hence to maximize the total load is to maximize the last integral:

$$\int\limits_0^1 R(x)dx \to \max \tag{11}$$

under the constraints:

$$0 \leq R \leq R_0 = \rho_0 L/(u_0 v), \qquad 0 \leq u \leq 1, \tag{12}$$

for the discharging rate and the solution of (8) with the same boundary conditions (6).

This problem can be classified as a constrained optimal control problem, which can be solved using advanced tools of control theory (see, for example, [3], [4]). However, in this simple case the solution can be found following the three steps outlined below, which require standard calculus tools and some geometric arguments.

1) The unconstrained general solution is found first for the special case $R(x) = C = \text{const}$, which means that the total load is homogeneously distributed in the segment $[0, 1]$: such a solution is also optimal if the concentration u remains below the Quality Standard for $C = R_0$.

2) If the unconstrained solution corresponding to $C = R_0$ violates the constraint, we show that the Total Load is maximized when the area under the graph u in the segment $[0, 1]$ is maximized.

3) Based on this, we find the optimal solution, the corresponding optimal discharge rate and the maximum Total Load under given constraints.

Results

The method outline in the previous section was applied to the special case $A = 0$, and to the general case $A \neq 0$, since the order of the equation and, therefore, the class of solutions are different. The first case correspond to a zero diffusivity: in physical terms, it could represent a system, such as a river, where the dispersion is accounted for mainly by the advective processes and diffusion is negligible.

Reaction-advection model

In this case, the model equation (8) takes the form

$$u' = -\Lambda u + R(x). \tag{13}$$

The initial value problem for this equation with $u(-\infty) = 0$ has a unique solution for any piecewise continuous (or even integrable measurable) distribution R being zero outside $[0, 1]$ (see eg. [1]). This solution has zero value for $x < 0$, defined by formula

$$e^{-\Lambda x} \int_0^x R(s) e^{\Lambda s} ds \tag{14}$$

for $0 \leq x \leq 1$ and

$$u(x) = e^{-\Lambda x} \int_0^1 R(s) e^{\Lambda s} ds$$

for $x \geq 1$.

In particular, $u(+\infty) = 0$ and the maximum value is attained in the interval $[0, 1]$. When the discharge rate R is constant, $R = C$, then solution (14) takes the form

$$u(x) = C(1 - e^{-\Lambda x})/\Lambda \tag{15}$$

The total load can be related to the solution by rearranging equation (13) and integrating over the segment [0, 1]:

$$\int_0^1 R(x)dx = \int_0^1 (u'(x) + \Lambda u(x))dx = u(1) + \Lambda \int_0^1 u(x)dx. \tag{16}$$

Eq. (16) tells us that the total load is given by the sum of two terms. The first is the pollution concentration at the end of the segment where discharge is allowed, $x = 1$, and the second is given by the area under the graph of the solution u on the interval $[0, 1]$.

Due to integration of inequalities at any point of the interval $[0, 1]$ this solution has a value not greater than the one provided by the distribution $R(x) \equiv R_0$. In particular, due to formulae (14) and (15) with $C = R_0$ on the interval $[0, 1]$ that gives inequality

$$e^{-\Lambda x} \int_0^x R(s)e^{\Lambda s}ds \leq R_0(1 - e^{-\Lambda x})/\Lambda. \tag{17}$$

The function on the right hand side of expression (3.5) increases monotonically on $[0, 1]$, and, when it does not violate constraint, that is

$$R_0(1 - e^{-\Lambda x})/\Lambda|_{x=1} = R_0(1 - e^{-\Lambda})/\Lambda \leq 1, \tag{18}$$

then the distribution $R \equiv R_0$ is optimal and the respective total load is R_0. This case is represented by the solid line in Fig. 1. Let us denote by R_c the *critical discharge rate* for constant distribution when the respective solution takes unit value at the right end $x = 1$:

$$R_c(1 - e^{-\Lambda})/\Lambda = 1 \quad \Rightarrow \quad R_c = \Lambda/(1 - e^{-\Lambda}) \tag{19}$$

This case is represented by the dashed curce in Fig. 1. Note that

$$R_c > \Lambda. \tag{20}$$

If $R_0 > R_c$ the solution corresponding to the distribution $R \equiv R_0$ exceeds the Quality Standard. However, since eq. (16) still holds, any solution which takes unit value at the right end $x = 1$ and maximizes the area under its graph on $[0, 1]$ is optimal, since it also maximizes the load.

It can easily be seen that the structure of such solution is unique: as shown by the dashed-dotted curve in Fig. 1, the solution coincides with the one provided by the maximum discharge rate $R \equiv R_0$ up to the point xc (change x0 in xc) where it meets the ecological constraint. Such point can be calculated from eq. (15) with $C \equiv R_0$:

$$1 = R_0(1 - e^{-\Lambda x_0})/\Lambda \qquad \Rightarrow \qquad x_0 = -\frac{1}{\Lambda}\ln(1 - \frac{\Lambda}{R_0}). \tag{21}$$

The logarithm here is well defined since $R_0 > R_c > \Lambda$. On the interval $[x_0, 1]$ we extend the solution as $u \equiv 1$. Due to $u' = 0$ here from the model equation (13) we find the respective discharge rate $R = \Lambda$, which is admissible again due to $R_0 > R_c > \Lambda$.

The above results can be summarized in the following theorem:

Theorem 1. *If $A = 0$ the optimal solution is provided by the distribution either $R(x) \equiv R_0$, $0 \leq x \leq 1$, when $R_0(1 - e^{-\Lambda})/\Lambda \leq 1$ or*

$$R(x) = \begin{cases} R_0, & 0 \leq x \leq -\frac{1}{\Lambda}\ln(1 - \frac{\Lambda}{R_0}) \\ \Lambda, & -\frac{1}{\Lambda}\ln(1 - \frac{\Lambda}{R_0}) < x \leq 1 \end{cases}, \tag{22}$$

in the other case.

Figure 1 illustrates this theorem.

In the second case, from Theorem 1 the total load is

$$TL = R_0 x_0 + \Lambda(1 - x_0) = \Lambda + (1 - \frac{R_0}{\Lambda})\ln(1 - \frac{\Lambda}{R_0}).$$

Thus the optimal total load in the case $A = 0$ is defined as

$$TL = \begin{cases} R_0, & 0 < R_0 \leq \Lambda/(1 - e^{-\Lambda}), \\ \Lambda + (1 - \frac{R_0}{\Lambda})\ln(1 - \frac{\Lambda}{R_0}), & \Lambda/(1 - e^{-\Lambda}) < R_0. \end{cases} \tag{23}$$

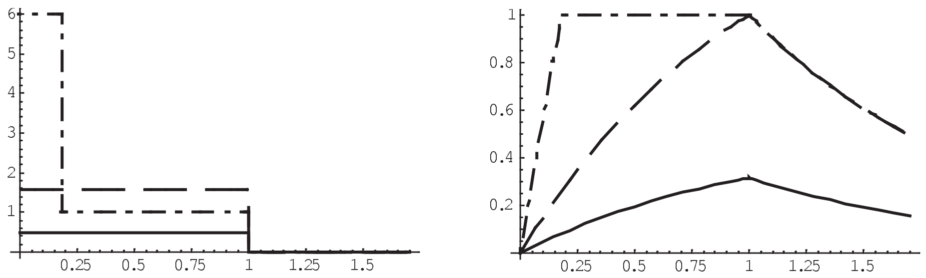

Figure 1: Distributions of the pollutant load (left) and concentrations simulated for the advection model ($A = 0$) in three cases: $R_0(1 - e^{-\Lambda})/\Lambda$ is less (solid line), equal (dashed line) and greater then 1 (dashed-dotted line), respectively.

Reaction-advection-diffusion model

In this section we present the results for the general case of nonzero eddy diffusion. As above, there exists a critical constant discharge rate R_c such that the rate $R \equiv R_0$ is optimal and corresponds to the the solution which meets exactly the Quality Standard at some point in the domain. As in the previous section, we find first this level and then explain the structure of optimal solution when this level is less then R_0.

With $A > 0$ and constant discharge rate $R = C$ the unique unconstrained solution of the boundary value problem (6), (8) can be found using basic calculus (see, for example, [1]). It is

$$u(x) = \begin{cases} C\left(1 + \frac{\lambda_2}{\lambda_1 - \lambda_2} + \frac{\lambda_1 e^{-\lambda_2}}{\lambda_2 - \lambda_1}\right) e^{\lambda_2 x}/\Lambda, & x < 0 \\ C\left(1 + \frac{\lambda_2 e^{\lambda_1 x}}{\lambda_1 - \lambda_2} + \frac{\lambda_1 e^{\lambda_2 (x-1)}}{\lambda_2 - \lambda_1}\right)/\Lambda, & 0 \le x \le 1 \\ C\left(1 + \frac{\lambda_2 e^{\lambda_1}}{\lambda_1 - \lambda_2} + \frac{\lambda_1}{\lambda_2 - \lambda_1}\right) e^{\lambda_1 (x-1)}/\Lambda, & 1 < x \end{cases} \tag{24}$$

where λ_1 and λ_2, $\lambda_1 < 0 < \lambda_2$, are the roots of the characteristic equation of equation (8). We show that below in Section .

This solution decreases at the infinity and attains its maximum only at one point $x_{max} = \lambda_2/(\lambda_2 - \lambda_1)$ which belongs to interval $(0, 1)$. Calculating this maximum $u_{max}(C)$ we get:

$$u_{max}(C) = C\left(1 - e^{\frac{\lambda_1 \lambda_2}{\lambda_2 - \lambda_1}}\right)/\Lambda = C\left(1 - e^{\frac{-\Lambda}{\sqrt{1+4A\Lambda}}}\right)/\Lambda$$

Therefore, the maximum depends linearly on C. By equatin the maximum to the Quality Standard, we can compute the critical discharge rate: e

$$1 = R_c\left(1 - e^{\frac{-\Lambda}{\sqrt{1+4A\Lambda}}}\right)/\Lambda \quad \Rightarrow \quad R_c = \Lambda/[1 - e^{-\Lambda/\sqrt{1+4A\Lambda}}]. \tag{25}$$

Remark 2. The last formula implies $\Lambda \in (0, R_0)$ when $R_0 > R_c$.

As in the reaction-advection model, a constant discharge rate would lead to breach the ecological constraint if R_0 exceeds the critical value R_c. For $R_0 > R_c$ the optimal discharge rate near both ends of the licensed area $[0, 1]$, namely, takes maximum possible value R_0 on some segments near the ends and constant value Λ on middle part. The calculations done below in the Section leads to the following statement:

Theorem 3. *For $A > 0$ and $R_0 > R_c$ the optimal discharge rate is*

$$R = \begin{cases} \Lambda, & x \in (x_1, 1 - x_2) \\ R_0, & x \in [0, x_1] \quad or \quad x \in [x_2, 1] \end{cases} \tag{26}$$

with

$$x_1 = -\frac{1}{\lambda_1}\ln\frac{R_0}{R_0 - \Lambda}, \qquad x_2 = \frac{1}{\lambda_2}\ln\frac{R_0}{R_0 - \Lambda}. \tag{27}$$

It leads to the solution which meats ecological (phase) constraint and provides the total load

$$TL = \sqrt{1 + 4A\Lambda}\frac{R_0 - \Lambda}{\Lambda}\ln\frac{R_0}{R_0 - \Lambda} + \Lambda. \tag{28}$$

Such structure of the optimal distribution was already observed in [2] for an another model. Logarithms here are well defined because due to Remark 2 we have $R_0 > \Lambda$ when $R_0 > R_c$. Direct calculation imply that the respective solution on interval $[0, 1]$ is

$$\begin{cases} \frac{R_0}{\Lambda} + (1 - \frac{R_0}{\Lambda})\frac{-\lambda_2 e^{\lambda_1(x-x_1)} + \lambda_1 e^{\lambda_2(x-x_1)}}{\lambda_1 - \lambda_2}), & 0 \le x \le x_1 \\ 1, & x_1 < x < x_2 \\ \frac{R_0}{\Lambda} + (1 - \frac{R_0}{\Lambda})\frac{-\lambda_2 e^{\lambda_1(x-1+x_2)} + \lambda_1 e^{\lambda_2(x-1+x_2)}}{\lambda_1 - \lambda_2}, & x_2 \le x \le 1 \end{cases}. \tag{29}$$

Again by direct calculation one can check up that the solution does not violate the constraint $u \le 1$. Figure 2 illustrate this theorem.

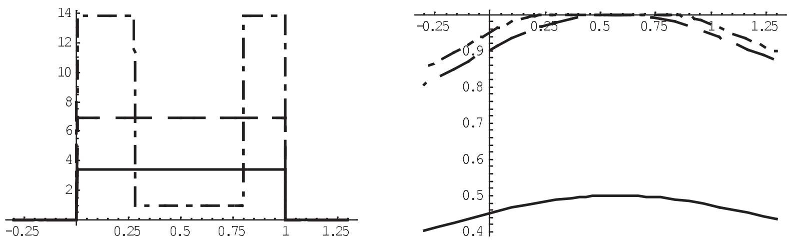

Figure 2: Distributions of the pollutant load (left) and concentrations (right) simulated using the advection model ($A > 0$) in three cases: $R_0 < R_c$ (solid line), $R_0 = R_c$ (dashed line) and $R_0 > R_c$ (dashed-dotted line)

Remark 4. For $R_0 = R_c$ the total load is R_c but for $R_0 > R_c$ it is greater then R_c. Indeed the second derivative of function $z \ln(1 + 1/z)$ with $z = (R_0 - \Lambda)/\Lambda$ is equal to $-1/[z(z+1)^2]$. It is negative for $z > 0$. Hence the first derivative $\ln(1 + 1/z) - 1/(z+1)$ of this function decreases on $z > 0$. But it has zero limit at infinity, and so it is positive on $z > 0$ and, in particular, on $R_0 > R_c$.

Remark 5. By unbounded increasing of constraint value R_0, that is $R_0 \to +\infty$, the total load has limit $\sqrt{1 + 4A\Lambda} + \Lambda$. The respective limit optimal distribution of pollution has point sources at the left and right ends of interval $[0, 1]$ with loads $-\Lambda/\lambda_1$ and Λ/λ_2, respectively, and homogeneous distribution of pollution inside the interval with value Λ.

Discussion of the results

The results demonstrated in the previous section indicate that control theory could be usefully employed for managing the emissions of a given pollutant into a water body, in compliance with a given Quality Objective, i.e. a threshold value of the concentration which should not be exceeded. In order to illustrate the possible relevance of the ideas developed in this paper, we present here two simple examples, in which we show the solutions of the model equation as the pollution level increases respectively, for the advection, Fig. 1, and the advection-diffusion model, Fig. 3. For the sake of simplicity, in figures we set $L = 1$ and $u_0 = 1$.

In both cases, the rate of increase in the concentration due to the presence of distributed sources of pollution is assumed to be constant, up to a critical value ρ_c, i.e. the value at which the steady-state concentration of u reaches the threshold. In this case, the increase in the concentration of the pollutant in the segment $[0, L]$ per unit of time, which is proportional to the total load per unit of time TL, is simply:

$$TL = B \int_0^L \rho dx = \rho L \tag{30}$$

in which ρ is the constant emission density and B is the constant lateral section of the system.

Once the critical level has been reached, a further increase in ρ would lead to breach the regulation in place. However, optimal control solution suggests that there are "smart" ways to redistribute the pollution along the segment L, in order to increase the value of TL even further and, at the same time, to comply with the QO.

Reaction-Advection model

In this case, as is shown by the continuous line on the right in Fig. 1, the concentration of the pollutant at steady state in the water body increases along the direction of the current and reaches its maximum value at the end of the segment $[0, L]$. The homogeneous distribution of the emissions along the segment represents also the "optimal" way to discharge the pollutant, until the constant emission rate reaches its critical value ρ_c, which is determined by the equation $u(L) = u_0$. From equation (14) we get:

$$1 = \frac{R_c(1 - e^{-\Lambda})}{\Lambda} = \frac{\rho_c(1 - e^{-\Lambda})}{u_0\lambda} \quad \Rightarrow \quad \rho_c = \frac{u_0\lambda}{1 - e^{-\lambda\tau}} \tag{31}$$

where $\tau = L/v$ is the transit time of water body on $[0, L]$. Denoting in (31)by $t_{1/2}$ the half-life time of the pollutant we get

$$\rho_c = \frac{u_0 \ln 2/t_{1/2}}{1 - e^{-\tau \ln 2/t_{1/2}}} \tag{32}$$

which leads to compute the critical value of the load per unit of time:

$$TL_c = \rho_c L.$$

As one can see from equation (32), the critical value depend on the QO, u_0, and on two parameters which can be taken as representative of the "assimilative capacity" of the section of the water body where the pollutant is discharged, namely the decay rate λ and the transit time, τ. Equation (32) can be simplified in two limit cases. If the transit time is much larger than the half-time, $\tau >> t_{1/2}$, the critical value approaches the limit:

$$\rho_c \approx u_0 \ln 2/t_{1/2}.$$

which means that assimilative capacity is mainly controlled by local processes.

On the other end, if $\tau << t_{1/2}$, the advection represents the main mechanism for the removal of the pollutant, since the critical value approaches the limit:

$$\rho_c \approx u_0/\tau.$$

If the load of pollutant is homogeneously distributed and $\rho > \rho_c$, the solution has the same shape, but $u(L)$ exceeds u_0. That means that the solution meet the QO at a certain point, x_c (=$x_{critical}$) within the licensed pollution area. This situation is shown by the dashed-dotted line on right in Fig. 1. The value x_c can be found from the equality $u(x_c) = 1$. After reintroducing the physical quantities, for $\rho = \rho_0$ that gives

$$\frac{R_0(1 - e^{-\Lambda x_c/L})}{\Lambda} = 1 \quad \Rightarrow \quad x_c = -\frac{L}{\lambda \tau} \ln{(1 - \frac{\lambda u_0}{\rho_0})} \tag{33}$$

In this case it would still be possible to comply with the regulation in place by redistributing the pollutant load along the segment. The optimal solution (=pollution distribution) is given by the piecewise continuous function, drawn by dashed-dotted line on the left in Fig. 1 and is obtained if we set two different constant pollution levels within the segment L. As one can see from the left graph of this figure the critical level ρ_c can be exceed in the segment $0 < x < x_c$, but, according with formula (22), in the remaining part the load must be kept at a certain level ρ_a, which depend on the assimilative capacity of the water body. In fact, according to this formula such constant level is the solution of the equation: $R = \Lambda$ from which, returning back to physical quantities, one gets:

$$\frac{\rho_a L}{u_0 \nu} = \frac{\lambda L}{\nu} \quad \Rightarrow \quad \rho_a = \lambda u_0. \tag{34}$$

It is easy to see, by direct substitution, that the emission rate ρ_a represents the solution of equation (13) when the spatial gradient vanishes, i.e for $du/dx = 0$. It is interesting to note that, once the QO has been fixed, this value does not depend on the transport mechanism but only on the rate of removal due to local processes, such as sedimentation, coprecipitation, chemical or biochemical reactions, biological uptake, etc..., which occur within the system.

The critical point, x_c, depends, instead, on both the decay rate and the transit time. Furthermore, as is clear from equation (33), it gets closer and closer to 0 as the difference between the critical emission rate and the one imposed on the system increases.

Another remarkable feature of the optimal solution is given by the fact that, by redistributing the pollution, the waterbody can tolerate a load TL_0 which is higher than TL_c, since $TL_0 = x_c(\rho_0 - \lambda u_0) + L\lambda u_0$ and for $\rho_0 > \rho_c$ we have

$$TL_0 > -\frac{L}{\lambda\tau} \ln\left(1 - \frac{\lambda u_0}{\rho_c}\right) \frac{\lambda u_0}{e^{\lambda\tau} - 1} + L\lambda u_0 = L\frac{\lambda u_0}{1 - e^{-\lambda\tau}} = L\rho_c = TL_c.$$

This expression can also easily be interpreted in geometrical terms, by looking at the areas of the rectangles shown in the graphs on the left in Fig. 1, and on the right part of this figure the respective concentrations simulated are drawn.

For the reaction-advection model the graphic of maximum total load as a function on emission density R, which is provided by the optimal spatial distribution, is drawn on the left in Fig. 3 by solid line. By such line on the right of this figure the graphic of the increasing in percents of the maximum total load in comparison with the best homogeneous one is depicted (also as a function on R). For the case of the reaction-advection-diffusion model, which is discussed below, such graphics in this figure is drawn by dashed line for $A = 1$ and by dashed-dotted for $A = 3$.

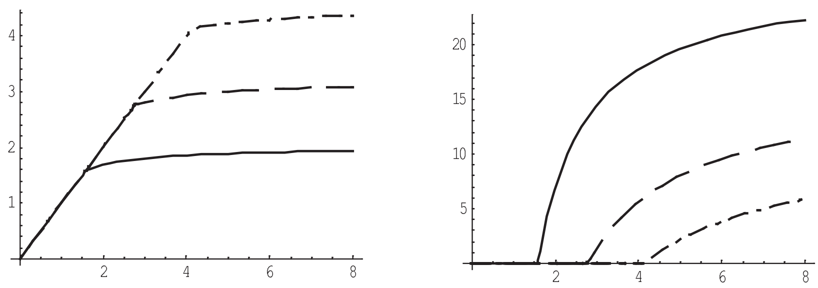

Figure 3: Comparison between the total loads for best homogenous solutions and the respective optimal solutions for $\Lambda = 1$ and $A = 0$ (solid line), $A = 1$ (dashed line) and $A = 3$ (dashed-dotted line)

The ratio between the maximum total load TL_0 provided by the optimal spatial distribution and the one corresponding the best homogenous distribution as a function on density R is shown on the left in Fig. 3, and on the right of this figure the increasing in percents of total load is shown as a function on R also. The graphics corresponding to the reaction-advection model are depicted by solid line.

Reaction-Advection-Diffusion model

In this case the analytical solution of model equation is slightly more complicated, but the basic ideas of the optimal solution can be grasped by looking at Fig. 2, which are similar to Fig. 1 and can be easily interpreted from a physical point view. In fact, a constant turbulent diffusion introduces a further mixing terms which, however, has no preferential direction and, therefore, the pollutant is be dispersed upstream the initial point of discharge, as well as downstream. As a result, as one can see from the continuous line on the left in Fig. 2, if the emission density is constant throughout the segment, the maximum value of the pollutant concentration is reached within the segment and not at its end, as in the case of the advection model.

As in the previous case, the homogeneous distribution of the total load represent the optimal distribution up to the maximum value reaches the QO, i.e. for $\rho_0 \leq \rho_c$. The solution corresponding to the optimal constant emission is represented in Fig. 3 by the solid and dashed lines when $\rho_0 < \rho_c$ and $\rho_0 = \rho_c$, respectively.

The critical emission density ρ_c is given by equation (19) which in the physical variables reads as:

$$\rho_c = \frac{\lambda u_0}{1 - e^{-\frac{\lambda L}{\sqrt{v^2+4\alpha\lambda}}}} \tag{35}$$

It is easy to see that, as expected, the introduction of diffusion leads to an increase in the critical value, and, therefore, of the total load, in comparison with the pure advection model, for which this value is λu_0. That is also illustrated by the left in Fig. 3 where the critical levels of density for A equals to 0, 1 and 3, respectively, are defined by points of diagonal at which the respective graphic leave it.

A further increase of a constant emission level above ρ_c would lead to breach the environmental regulation. In this case on the graphic of optimal pollution concentration there appears horizontal arc as in the previous one (Fig. 2, right, dashed-dotted line). But here the solution is differentiable and the pollution concentration has zero derivatives at the ends of this arc, e.c its graphic is tangent to this arc at the ends in contrast with the case of zero eddy diffusion.

The optimal solution (29) it is obtained by imposing two different levels of constant emissions, in accordance with (26), which in physical units reads as:

$$\rho(x) = \begin{cases} \lambda u_0, & x \in [Lx_1, L(1-x_2)] \\ \rho_0, & x \in [0, Lx_1] \quad \text{or} \quad x \in [Lx_2, L] \end{cases} \tag{36}$$

where x_1 and x_2 are defined by formula (27).

Fig. 3 illustrates the comparison of the respective total loads as we discussed above.

It is interesting to note the introduction of turbulent diffusion does increase the maximum daily load which can be tolerated, but does not affect the low-emission level which has to be respected, in order to be able to discharge more pollutant at the two ends of the system. Such level depend, as in the advection model, only on the rate of internal processes which can lead to the removal of the pollutant and, therefore, on the type of pollutant and type of system. It is a site-specific constraint which it would be very important to estimate with accuracy, in order to manage the pollution discharges in a cost effective manner.

Appendix for case with diffusion

Here we initially get some property of optimal solution and then use them and geometrical reasons to find the optimal solution.

Uniqueness and positivity of pollution concentration

Under the notion of applications R is reasonable to be assumed a piecewise-continuous function. For such

Proposition 6. *For $A > 0$ and any piecewise-continuous function R boundary-value problem (8), (6) has unique solution.*

Proof. If there are two solutions then the difference of them satisfies the homogeneous equation (8) and the same boundary conditions. The general solution of this equation has the form

$$C_1 e^{\lambda_1 x} + C_2 e^{\lambda_2 x}, \tag{37}$$

where $\lambda_{1,2} = \frac{1 \pm \sqrt{1+4A\Lambda}}{2A}$ are the roots of the characteristic equation, and C_1 and C_2 are arbitrary real constants. Substituting to this solution boundary conditions we immediately get $C_1 = C_2 = 0$. So there could be only one solution of problem (8), (6).

To prove the existence it is sufficient to find explicit formula of the solution. Outside the the interval $[0,1]$ our equation is homogeneous and the formula (37) provides its general solution. Satisfying the boundary conditions we arrive to the solution

$$\begin{cases} C_1 e^{\lambda_1 x}, \text{ while } x < 0, \\ C_2 e^{\lambda_2 x}, \text{ while } x > 1. \end{cases} \tag{38}$$

outside the interval $[0,1]$.

Our equation (8) is of second order and the emission density function is piecewise-continuous. Consequently its solution has to be differentiable, and from form (38) get that the following equalities must be satisfied at the ends of $[0,1]$:

$$u'(0) = \lambda_1 u(0), \qquad u'(1) = \lambda_2 u(1). \tag{39}$$

Thus it is sufficient to find the solution of boundary value problem (8), (39). General solution of the equation (8) has the form

$$C_1 e^{\lambda_1 x} + C_2 e^{\lambda_2 x} + f(x),$$

where C_1 and C_2 are arbitrary real constants and f is some partial solution of this equation. Substituting this solution to condition (39) we get system of linear equation on constants C_1 and C_2:

$$\begin{cases} C_1(\lambda_1 - \lambda_2)e^{\lambda_1} = \lambda_2 f(1) - f'(1), \\ C_2(\lambda_2 - \lambda_1) = \lambda_1 f(0) - f'(0). \end{cases}$$

which due to $\lambda_1 - \lambda_2 > 0$ has unique solution:

$$C_1 = \frac{\lambda_2 f(1) - f'(1)}{(\lambda_1 - \lambda_2)e^{\lambda_1}}, \quad C_2 = \frac{\lambda_1 f(0) - f'(0)}{\lambda_2 - \lambda_1}.$$

Consequently our boundary-value problem has unique solution. □

Proposition 7. *For $A > 0$ the solution of boundary-value problem (8), (6) is positive on the interval $[0, 1]$, and so on the whole real line, if a piecewise-continuous nonnegative function R is nonnegative and delivers nonzero total load (11).*

Proof. Assume contrary, that the solution u has non-positive values on the interval $[0, 1]$ while $R \geq 0$ and $TL > 0$. Due to continuity of the solution and its zero limit at the infinity this assumption implies the existence of its non-positive minimum.

When the minimum is negative then at point x_0 of such a minimum we have $u'' \geq 0$, $u' = 0$, $u < 0$, as it is easy to see (we consider right and left side second derivatives if it does not exist). Hence, near this point but outside it the left hand side of the equation (8) is positive, while the right one is not. Thus the equation is not satisfied, we arrive to contradiction, and so under our assumption the minimum could be only zero.

When this minimum is zero denote by x_0 the minimum value of $x \in [0, 1]$, at which the solution vanishes. We have condition $u'(x_0) = u(x_0) = 0$ because the solution is differentiable and attains its minimum at x_0.

Using these conditions, form (37) of the solution of homogeneous equation (8) and variation constant method we get the following formula for the solution satisfying the condition:

$$u(x) = \frac{1}{\lambda_1 - \lambda_2} \int\limits_{x_0}^{x} R(t)(-e^{\lambda_1(x-t)} + e^{\lambda_2(x-t)})dt.$$

Due to $\lambda_2 < 0 < \lambda_1$ the coefficient by integral is positive and the integrant is negative and positive when R is positive and t either greater or less then x_0, respectively. Hence the solution u is non-positive and takes negative values inside $(0, 1)$ due to $R \geq 0$ and delivers nonzero total load. We again arrive to contradiction which finishes the proof.

Thus the solution is positive if $R \geq 0$ delivers nonzero total load. □

Proof of Theorem 3

Inside interval $[0,1]$ for a constant distribution $R = C$ the general solution of model equation is $u(x) = C_1 e^{\lambda_1 x} + C_2 e^{\lambda_2 x} + C/\Lambda$. Substituting it to boundary conditions (39) we find the constants

$$C_1 = \frac{\lambda_2}{\lambda_1 - \lambda_2} \cdot \frac{C}{\Lambda} e^{-\lambda_1}, \quad C_2 = \frac{\lambda_1}{\lambda_2 - \lambda_1} \cdot \frac{C}{\Lambda}.$$

Thereby on the interval the needed solution has the form

$$u(x) = C \left(1 + \frac{\lambda_2 e^{\lambda_1 (x-1)}}{\lambda_1 - \lambda_2} - \frac{\lambda_1 e^{\lambda_2 x}}{\lambda_1 - \lambda_2} \right) / \Lambda.$$

The extension of this solution to real line is obvious and has unique maximum located on $(0,1)$. Its maximum value $u_{max}(C)$ depends on C linearly as it easy to see.

Proposition 8. *When $u_{max}(R_0) > 1$ any admissible discharge distribution is not optimal if it leads to model equation solution with maximum being less then ecological constraint value* 1.

To prove that assume contrary, namely, that for an optimal discharge rate R the maximum of respective solution u is less then 1. The distribution R does not equal identically R_0 because the constant distributions R_0 is not admissible. Consider the perturbation $\tilde{R}, \tilde{R} = R + (R_0 - R)\theta$, with a small positive parameter θ and the respective solution $\tilde{u}$ of our model equation on the interval $[0,1]$ with perturbed boundary conditions

$$\tilde{u}'(0) = \lambda_1 \tilde{u}(0), \quad \tilde{u}(0) = u(0) + \delta.$$

The solution $\tilde{u}$ is differentiable with respect to θ and δ [1], and so we can present it in the form

$$\tilde{u} = u + \theta u_1 + \delta u_2 + ...,$$

with "dots" staying for the terms of higher order with respect to θ and δ, and u_1 and u_2 being the solutions of Cauchy problems, respectively

$$A u_1'' - u_1' - \Lambda u_1 = -(R_0 - R(x)), \quad u_1'(0) = u_1(0) = 0, \tag{40}$$

$$u_2'' - u_2' - \Lambda u_2 = 0, \quad u_2'(0) = \lambda_1, \quad u_2(0) = 1, \tag{41}$$

For sufficiently small values of θ, δ new solution also does not take the value 1 due to its continuous dependence on these values and x [1]. So it could be extended on the interval $[0,1]$ as admissible if we satisfy the boundary condition at $x = 1$. Due to $u'(1) = \lambda_2 u(1)$ one needs to have

$$(\theta u_1' + \delta u_2' + ...)\,|_{x=1} = \lambda_2 \,(\theta u_1 + \delta u_2 + ...)\,|_{x=1} \tag{42}$$

Substituting solutions of Cauchy problems (40) and (41) instead of u_1 and u_2, respectively, we find that equality (42) is satisfied when

$$\delta = \left[\theta \lambda_2 \frac{R_0}{\Lambda} + ...\right] \frac{1}{(\lambda_1 - \lambda_2)e^{\lambda_1}}$$

Hence for a sufficiently small positive θ there is an admissible solutions provide by distribution $\tilde{R}$ with greater total load then for the initial one. But that contradicts with the optimality of the initial solution and proves the proposition.

Thus an optimal solution has to meet constraint. Due to differentiability of any solution of model equation (with measurable bounded distribution R) the derivative of admissible solution u at a point with $u = 1$ should be zero, otherwise the solution violates the constraint near the point. Denote by R and optimal distribution, and by x_1, x_2 the least and greatest value of x at which the respective solution u takes value 1.

Proposition 9. *If inside the interval* $[x_1, x_2]$ *we modify the pair* $\{R, u\}$ *by changing it on the pair* $\{\Lambda, 1\}$ *then the new pair is admissible and provides greater total load, namely,*

$$\int_{x_1}^{x_2} R(x)dx < \Lambda(x_2 - x_1)$$

if u *is not identically* 1 *on the interval. In particular an optimal solution has only one boundary arc being maybe just contact point.*

The statement is trivial when $x_1 = x_2$. Let $x_1 < x_2$. Due to $0 \le R \le R_0$, $0 < u \le 1$ and u is not identically 1 on interval $[x_1, x_2]$ we get

$$0 = A \int_{x_1}^{x_2} u''(x)dx = \int_{x_1}^{x_2} (u'(x) + \Lambda u(x) - R(x))dx =$$

$$= 0 + \Lambda \int_{x_1}^{x_2} u(x)dx - \int_{x_1}^{x_2} R(x)dx < \Lambda(x_2 - x_1) - \int_{x_1}^{x_2} R(x)dx$$

and, consequently, the proposition statement is true.

Now let us prove Theorem 3. It is sufficient to show that for left and the right entry points x_1 and x_2, respectively, the optimal distribution has to have maximal value R_0 on the intervals $[0, x_1)$ and $(x_2, 1]$. Consider the case of the first interval (an another one is analyzed analogously).

Due to model equation for the load TL_1 provided by interval $[0, x_0]$ with $u(x_0) = 1$ we have

$$\int_0^{x_0} R(x)dx = \int_0^{x_0} [\Lambda u(x) + u'(x) - Au''(x)]dx =$$

$$= \Lambda \int_0^{x_0} u(x)dx + 1 - u(0) - Au'(0) = \Lambda \int_0^{x_0} u(x)dx + [1 - (1 + \lambda_1 A)u(0)]$$

The value in the square brackets is defined by the $u(0)$, that is by the concentration level at the left end. When this level is fixed then an optimal solution u with such a level has to provide the maximum of integral $\int_0^{x_0} u(x)dx$.

But geometrically the form of this solution u is obvious (see Fig. 4).Its pollution density is zero in the beginning, $x \in [0, a]$, maximal R_0 in the middle, $x \in [a, b]$, and has value Λ in the rest part of $[0, x_0]$.

Trying now to select the best one from the solutions of this type by the change of initial level we immediately get the load TL_1 of the last solution could be increased on the value $a\Lambda$ by the shift of its arc corresponding to the density R_0 to left on the distance a (see Fig. 5).

Consequently the solution from Theorem 3 is optimal, and it is unique optimal solution due to the reasons above.

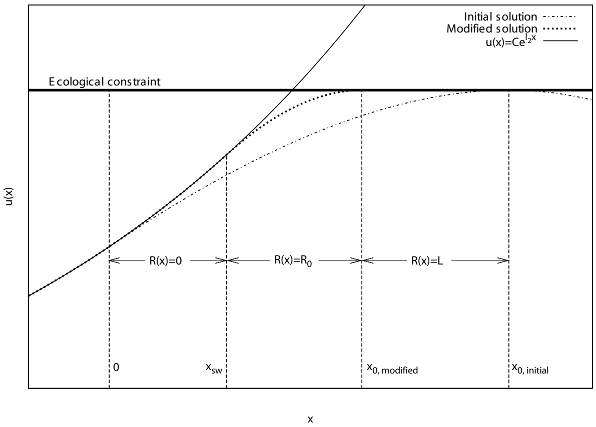

Figure 4: Solution with given level $u(0)$ and maximum total load on $[0, x_0]$.

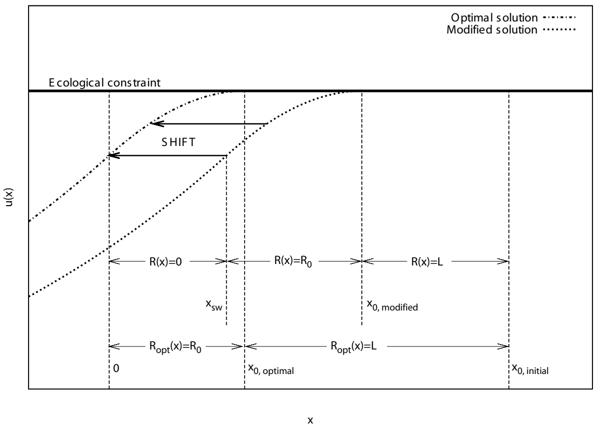

Figure 5: Optimal solution on $[0, x_0]$.

References

[1] Arnold V.I. - *Ordinary differential equations*// Cambridge: m.i.t. press, 1973, 280 pp.

[2] Brigolin D., Davydov.A.A., Pastres R., Petrenko I. - *Optimization of shellfish production carrying capacity at a farm scale*//Applied Mathematics and Computation, Volume 204, Issue 2, 15 October 2008, Pages 532-540.

[3] Hartl R.F., Sethi S.P., Vickson R.G. - *A survey of the maximum prin-*

ciples for optimal control problems with state constraints// Society for Industrial and Applied Mathematics vol.37, No2, 1995, 181-218.

[4] Maurer H., On optimal control problems with bounded state variables and control appearing linearly//SIAM J. Control and Optimization 15 (1977), 345-362.