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POLLUTION CONTROL METHODS

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Abstract: Methods for estimating the mean concentration of pollutants in ecologically sensitive zones and preventing their dangerous levels through a control of emission rates of sources are described. The methods are based on the adjoint approach taking advantage the dual (direct and adjoint) pollution concentration estimates in certain zones. The direct estimates use the solutions of pollution transport model allow performing complete analysis of ecological situation. On the other hand, the adjoint estimates depend explicitly on the number, positions and emission rates of the sources and the initial distribution of pollutants in the region. In the last estimates, the solutions of adjoint problem serve as weight function which provides valuable information on the contribution of each source and initial data to the pollution of the zone. This makes them very efficient in studying the model response to variations in the emission rates and initial conditions, and in developing control strategies.

A few control strategies, both non-optimal (sufficient) and optimal, have been developed. Each control strategy develops quantitative criteria with the aim to avoid violations of existing sanitary norm through reductions in the emission rates of sources. Such criteria are designed taking into account the processes of dispersion and transformation of pollutants, the number of point sources to control, their locations and corresponding sanitary norms. The methods are illustrated by simple examples. An optimal control strategy based on

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the adjoint method is also applied for cleaning aquatic zones contaminated with biofilm (remediation) or oil (bioremediation).

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1. Introduction

The phenomenon of pollution in any environment is the result of a huge global population with a modern lifestyle that demands and consumes a large amount of goods and services. For example, due to this demand which has presented a steady increase in recent decades, large volumes of raw materials and fossil fuels are transformed to various pollutants released into the atmosphere [11, 30]. The environment has mechanisms to dilute and assimilate these pollutants and returning them to nature [55]; however, during the last century, anthropogenic activities emit into the atmosphere at short intervals, such large volumes of substances in confined areas (cities, industrial parks, etc.) that the mechanisms of assimilation do not have time to recycle the excess chemicals and to clean the atmosphere. The result is the accumulation of different primary pollutants, leading to the generation of secondary species [35, 55, 67], which form a mixture that produces a variety of damages to humans and ecosystems [6].

Each pollutant, depending on its concentration and toxicity causes various health problems [22], from respiratory discomfort in the healthy people to the increase in mortality among vulnerable populations (cardiac patients, children, elderly persons, etc.). In any case, contamination is a factor that diminishes the quality of life of human beings. Unfortunately, the impact of mixing of pollutants in ecosystems can be not only local, as in the case of photochemical smog [5], but also regional, as in the acid precipitation [4, 53], or global, as the phenomenon of destruction of the ozone layer and global climate change [21, 51, 54].

Therefore, it is important to design methods of controlling emissions and reducing the concentration of harmful substances to acceptable health standards [50]. To this end, mathematical models of pollutant dispersion as well as their adjoint models are used [16, 25, 27-29, 32, 34, 36-39, 41-44, 59].

This approach permits us to realize the computer-simulation of concentrations of various primary and secondary pollutants in a region [12, 17-19, 48, 57, 59, 64, 65], and thereby identify the domains where the emissions have a greater impact. The method allows identifying the main sources responsible for

excessive pollution of a selected zone (residential region, park, forest, etc.). In particular, it can be used for the evaluation of pollution level due to oil spill [9, 10, 58, 60, 63], for estimating parameters which describe the source location and strength [23, 24], for the detection of the industrial plants which violate the emission rates, prescribed by some control strategy [63], for the reconstruction of an unknown number of contaminant sources [70], or for the optimal location of a new industrial enterprise in the sense that its operation will not violate health standards in ecologically most important zones [31, 32, 66]. The method can also be used to install safety devices in high-risk areas to prevent accidents or unauthorized discharges of contaminants and design emission control strategies for already existing industry [20, 41, 42, 49, 68, 69, 71].

This paper presents a technique based on using dispersion models and corresponding adjoint models, to estimate pollution levels and generate some strategies to control emission rates. These strategies include a limitation of emissions of pollution sources in order to meet sanitary norms. Because the sanitary standards represent time averages, the proposed control strategies are aimed at reducing the average concentration of pollutants in a given time interval and region, to an acceptable level. Some examples on the application of control strategies are considered in cases where the dispersion model predicts a violation of sanitary norms.

In general, there are two approaches to monitor and control the emission of pollutants and protect the environment in large industrial regions. The first approach, called "technological path" uses "green" technologies in order to maintain the lowest level of emissions of dangerous pollutants. The second approach consists in establishing various criteria for controlling the emission rates of pollutant sources, and presents a significant mathematical interest.

In order to illustrate principal mathematical ideas of the control methods, we will often use a simple two-dimensional (vertically integrated) transport model of passive pollutants, i.e. the substances, whose chemical reactions are described by means of a linear law. Of course, all the suggested methods can also be applied to a three-dimensional pollution transport model. On the other hand, the experience gained in the development of such strategies for the atmosphere has allowed expanding the scope of their application [1-3, 7, 14] for cleaning (remediation) aquatic systems polluted by biofilms or petroleum [45, 47].

2. A Limited Area Pollution Transport Model

In order to simplify the study, we will often consider a two-dimensional (vertically averaged) problem of pollutant transport. The three-dimensional problem is applied here only in the numerical experiment on the remediation of contaminated aquatic systems. Besides, we will always consider this process separately from the fluid dynamics problem, supposing that the transport velocity and other dynamic parameters of problem are known.

Initial and boundary conditions. Let D be a two-dimensional limited area with boundary S that contains N industries located at points $\mathbf{r}_i = (x_i, y_i)$, $i = 1, 2, ..., N$. Denote by $\phi(\mathbf{r}, t)$ the concentration of a contaminant in point $\mathbf{r} = (x, y)$ and moment $t > 0$. In order to study the propagation of the contaminant in time interval $(0, T)$, we consider in the domain D and time interval $(0, T)$ the advection-diffusion-reaction equation

$$\frac{\partial}{\partial t}\phi + \overrightarrow{U} \cdot \nabla\phi + \sigma\phi - \nabla \cdot (\mu\nabla\phi) = f(\mathbf{r}, t), \tag{1}$$

where

$$f(\mathbf{r}, t) = \sum_{i=1}^{N} Q_i(t)\delta(\mathbf{r} - \mathbf{r}_i), \tag{2}$$

$Q_i(t)$ is the emission rate of the ith industry, $\mu(\mathbf{r}, t) > 0$ is the turbulent diffusion coefficient, ∇ is the 2D gradient, and $\delta(\mathbf{r} - \mathbf{r}_i)$ is the Dirac function. The parameter $\sigma(\mathbf{r}, t) > 0$ characterizes the speed of exponential decay of $\phi(\mathbf{r}, t)$ due to various physical and chemical processes. Numerical experiments with equation (1) show that the parameterisation $\sigma\phi$ is quite good in the case of such contaminants as CO, SO_2 Pb, C, etc. [56].

The wind velocity vector $\overrightarrow{U}(\mathbf{r}, t) = \{u(\mathbf{r}, t), v(\mathbf{r}, t)\}$ is assumed to be known from observations or some dynamic model and to satisfy the continuity equation

$$\nabla \cdot \overrightarrow{U} = 0. \tag{3}$$

The equation (1) is solved with initial condition at $t = 0$:

$$\phi(\mathbf{r}, 0) = \phi^0(\mathbf{r}). \tag{4}$$

Since the pollution flux through the open boundary S of limited area D is unknown, the errors made in determining the flux will propagate inside the domain by advection and diffusion, and perturb or destroy the exact solution. In addition, errors in the initial condition (4) and emission rates $Q_i(t)$ can also

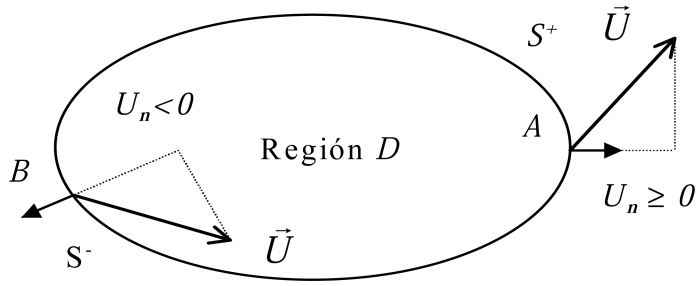

Figure 1: Limited area D with open boundary $S = S^+ + S^-$ of problem (1)-(5).

distort the solution. In order to pose the problem well, it is important to select boundary conditions that are correct both physically and mathematically [32, 34]. To this end, we introduce the projection $U_n = \overrightarrow{U} \cdot \overrightarrow{n}$ of velocity $\overrightarrow{U}$ on the unit external normal $\overrightarrow{n}$ to the boundary S of domain D, and divide the boundary into the "inflow" part S^- (where $U_n < 0$, and the pollution flux is directed inside area D) and "outflow" part S^+ (where $U_n \geq 0$, and the pollution flux is directed outside area D) (Figure 1). Then we take the following boundary conditions:

$$\mu \nabla \phi \cdot \overrightarrow{n} - U_n \phi = 0 \quad \text{at} \quad S^- \quad , \qquad \mu \nabla \phi \cdot \overrightarrow{n} = 0 \quad \text{at} \quad S^+, \tag{5}$$

see [34, 59]. It is shown in [64] that problem (1)-(5) is well posed according to Hadamard [15], that is, it possesses unique solution, which continuously depends not only on the initial distribution $\phi^0(\mathbf{r})$, but also on the number N, emission rates $Q_i(t)$ and positions $\mathbf{r}_i$ of the industries.

Integral equations. By integrating equation (1) over domain D and taking into account conditions (3) and (5) we obtain the balance equation for the total mass of contaminant:

$$\frac{\partial}{\partial t} \int_D \phi d\mathbf{r} = \sum_{i=1}^{N} Q_i(t) - \int_{S^+} U_n \phi dS - \int_D \sigma \phi d\mathbf{r}. \tag{6}$$

And multiplying equation (1) by $\phi(\mathbf{r}, t)$ and integrating the result obtained over domain D, we get another integral equation:

$$\frac{\partial}{\partial t} \int_D \phi^2 d\mathbf{r} = 2 \sum_{i=1}^{N} Q_i(t) \phi(\mathbf{r}_i, t) - \int_S |U_n| \, \phi^2 dS - 2 \int_D (\sigma \phi^2 + \mu \, |\nabla \phi|^2) d\mathbf{r}. \tag{7}$$

According to (6) y (7), both the total concentration $\int_D \phi d\mathbf{r}$ and solution norm $\|\phi\| = \left(\int_D \phi^2 d\mathbf{r}\right)^{1/2}$ increase due to non-zero emission rates $Q_i(t)$, and at the same time decrease because of processes of dissipation ($\sigma > 0$, $\mu > 0$) and non-zero adjective pollution flux through the boundary S of domain D. If, in addition, there is no dissipation ($\sigma = 0$, $\mu = 0$) and $U_n = 0$ everywhere at the boundary S, then both the integrals are conserved with time:

$$\frac{\partial}{\partial t}\int_D \phi d\mathbf{r} = 0\ , \quad \frac{\partial}{\partial t}\|\phi\| = 0. \tag{8}$$

Although the conservation laws (8) are obtained under artificial boundary conditions, they (as well as the balance equations (6) and (7)) are very useful in testing numerical algorithms and computational programs [59].

Pollution sources. The problem forcing $f(\mathbf{r}, t)$ depends on the type of pollution source. For example, in the case of N industrial plants located in D (Figure 2a) we take $f(\mathbf{r}, t)$ in form (2). And if instead of point sources, we consider the sources, continuously distributed along the main city roads R_i (Figure 2b), then

$$f(\mathbf{r}, t) = \begin{cases} Q_i(\mathbf{r}, t) & \text{if } \mathbf{r} \in R_i \\ 0 & \text{if } \mathbf{r} \notin R_i \end{cases} \quad (i = 1, 2, ..., N)\ , \tag{9}$$

where $Q_i(\mathbf{r}, t)$ is a continuous function that describes the emission rate of a contaminant along the road R_i, [62]. The form (9) is also used to define superficially distributed sources (for example, in case of a conflagration). However, it should be noted that the emission rates $Q_i(\mathbf{r}, t)$ continuously distributed along some line R_i (or over some area) can also be included in the model in discrete form (2) by means of division of the line (or the area) into small parts with subsequent discretization of function $Q_i(\mathbf{r}, t)$ [43, 62].

Figure 3 shows the importance of winds in the distribution of carbon monoxide concentrations calculated with the model (1)-(5) in Guadalajara City with climatic winds of rainy season (a) and dry season (b). The vehicular sources located along the main roads were used in discrete form (2), see [62].

3. Adjoint Approach

Despite the fact that the solution of problem (1)-(5) allows us to know the pollutant concentration in any point of domain $D \times (0, T)$ (see Figure 3), the use of such solutions is not efficient way to answer such important question as the extent to which this or that source is responsible for the pollution of a

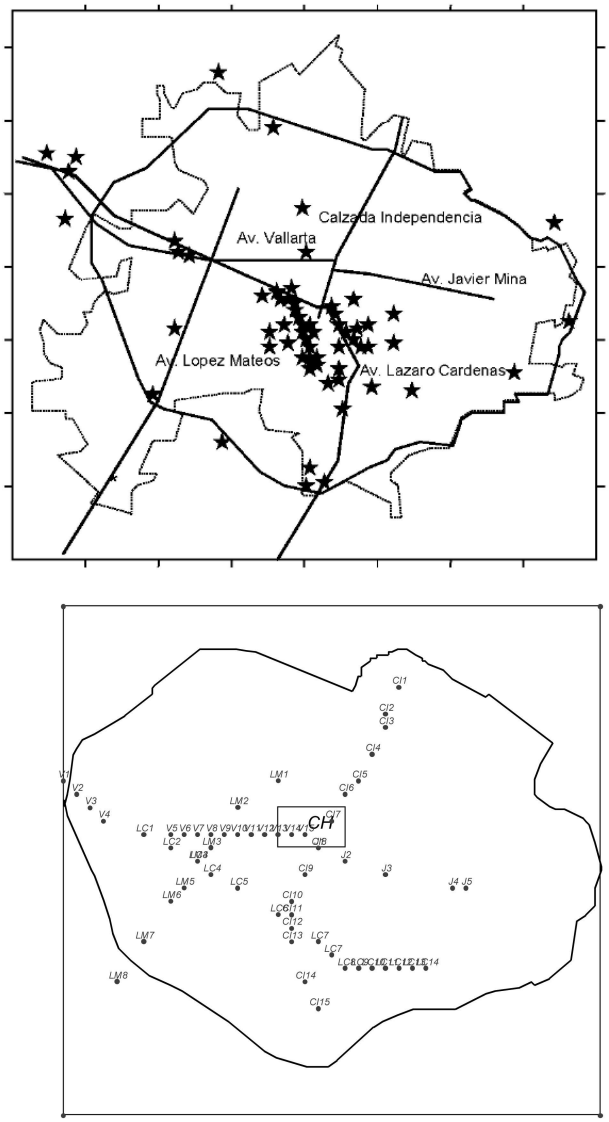

Figure 2: Main roads of Guadalajara City, and positions of 52 principal industries that burn fossil fuels and emit sulfur dioxide (a); discretization of vehicular sources of CO (b).

specific zone. It is much easier to answer this question with the help of adjoint method, widely used in the model sensitivity study and control theory [33]. The usefulness of this method lies in the fact that solutions of the adjoint problems

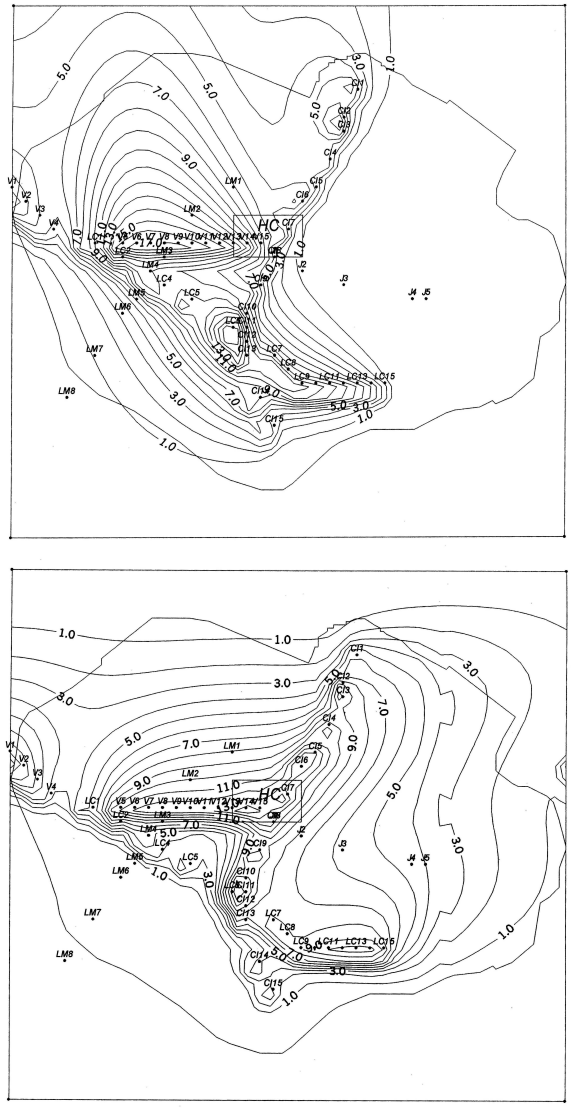

Figure 3: Isolines of the concentration of CO calculated at $t = 180$ *min* with model (1)-(5) using climatic winds of rainy season (a), and dry season (b).

are information functions [26].

Adjoint Transport Model. The adjoint transport model in the domain

D (Figure 1) and time interval is established by using the Lagrange identity and the concept of adjoint operator with respect to the operator of model (1)-(5) [32, 34]:

$$-\frac{\partial}{\partial t}g - \overrightarrow{U} \cdot \nabla g + \sigma g - \nabla \cdot (\mu \nabla g) = p(\mathbf{r}, t) \quad \text{in } D \times (0, T) \tag{10}$$

$$g(\mathbf{r}, T) = 0 \quad \text{in } D \tag{11}$$

$$\mu \nabla g \cdot \overrightarrow{n} = 0 \quad \text{at} \quad S^- \quad , \quad \mu \nabla g \cdot \overrightarrow{n} + U_n g = 0 \quad \text{at} \quad S^+. \tag{12}$$

Note that in equation (10), the wind velocity $\overrightarrow{U}(\mathbf{r}, t)$ and coefficients $\mu(\mathbf{r}, t)$ and $\sigma(\mathbf{r}, t)$ are the same as in equation (1). Let us compare the original problem (1)-(5) with adjoint problem (10)-(12) in the case when $f(\mathbf{r}, t) \equiv 0$ and $p(\mathbf{r}, t) \equiv 0$. It is easy to see that after substitution $t' = T - t$, equation (10) differs from equation (1) only in the sign of velocity $\overrightarrow{U}$. Therefore in the problems (1)-(5) and (10)-(12), the inflow and outflow parts S^- and S^+ are swapped. This fact explains the differences of the boundary conditions (5) and (12). It also shows that the adjoint problem is well posed only if it is solved in the opposite time direction: from $t = T$ to $t = 0$. That is why we take "initial" condition (11) at the moment $t = T$.

Duality Principle. We now determine the forcing $p(\mathbf{r}, t)$ of adjoint problem and show the role of its solution $g(\mathbf{r}, t)$. Suppose we need to know the mean concentration of contaminant $\phi(\mathbf{r}, t)$ in some ecologically sensible zone $\Omega \subset D$ and time interval $(T - \tau, T)$ of longitude τ. Let $\omega(\mathbf{r}, t)$ be a positive function in the domain $\Omega \times (T - \tau, T)$ such that

$$\int_{T-\tau}^{T} \int_{\Omega} \omega(\mathbf{r}, t) d\mathbf{r} dt = 1. \tag{13}$$

Then the integral

$$J_\omega(\phi) = \int_{T-\tau}^{T} \int_{\Omega} \omega(\mathbf{r}, t) \phi(\mathbf{r}, t) d\mathbf{r} dt \tag{14}$$

represents an average concentration of contaminant $\phi(\mathbf{r}, t)$ in zone Ω and interval $(T - \tau, T)$.

Let us subtract the equation (10) pre-multiplied by $\phi(\mathbf{r}, t)$ from the equation (1) pre-multiplied by $g(\mathbf{r}, t)$, and then integrate the result obtained over domain $D \times (0, T)$. Taking into account the initial and boundary conditions (4)-(5) and (11)-(12) we obtain the duality principle [34]:

$$\int_0^T \int_D p(\mathbf{r},t)\phi(\mathbf{r},t)d\mathbf{r}dt = \sum_{i=1}^{N} \int_0^T g(\mathbf{r}_i,t)Q_i(t)dt + \int_D g(\mathbf{r},0)\phi^0(\mathbf{r})d\mathbf{r}. \quad (15)$$

If the forcing $p(\mathbf{r},t)$ of adjoint problem is defined as

$$p(\mathbf{r},t) = \begin{cases} \omega(\mathbf{r},t)\ , & \text{if } (\mathbf{r},t) \in \Omega \times (T-\tau,T) \\ 0 & \text{otherwise} \end{cases}, \quad (16)$$

then (15) leads to another estimate of average concentration of contaminant $\phi(\mathbf{r},t)$ in zone Ω and interval $(T-\tau,T)$:

$$J_\omega(\phi) \equiv \int_{T-\tau}^{T} \int_\Omega \omega(\mathbf{r},t)\phi(\mathbf{r},t)d\mathbf{r}dt = \sum_{i=1}^{N} \int_0^T g(\mathbf{r}_i,t)Q_i(t)dt + \int_D g(\mathbf{r},0)\phi^0(\mathbf{r})d\mathbf{r}. \quad (17)$$

In particular case that $\omega(\mathbf{r},t) = 1/(\tau\,|\Omega|)$ in the domain $\Omega \times (T-\tau,T)$, where $|\Omega|$ is the area of Ω, the formulas (14) and (17) allow us to estimate the mean concentration of $\phi(\mathbf{r},t)$ in the space-time domain $\Omega \times (T-\tau,T)$ by means of direct estimate

$$J(\phi) = \frac{1}{\tau\,|\Omega|} \int_{T-\tau}^{T} \int_\Omega \phi(\mathbf{r},t)d\mathbf{r}dt, \quad (18)$$

or adjoint estimate [34]:

$$J(\phi) = \sum_{i=1}^{N} \int_0^T g(\mathbf{r}_i,t)Q_i(t)dt + \int_D g(\mathbf{r},0)\phi^0(\mathbf{r})d\mathbf{r}. \quad (19)$$

Thus, the forcing $p(\mathbf{r},t)$ of adjoint problem (10)-(12) characterizes the average concentration $J(\phi)$ in $\Omega \times (T-\tau,T)$. By (19), the concentration $J(\phi)$ in zone Ω explicitly depends on the emission rates $Q_i(t)$ and initial distribution $\phi^0(\mathbf{r})$ in D, besides, the solution $g(\mathbf{r},t)$ of adjoint problem serves as a weight function that determines the contribution of each source $Q_i(t)$ and initial pollution level $\phi^0(\mathbf{r})$ into $J(\phi)$ in Ω.

It should be noted that the role of initial distribution of contaminant $\phi^0(\mathbf{r})$ decreases when the interval $(0,T-\tau)$ increases [57]. Indeed, according to (16), $p(\mathbf{r},t) \equiv 0$ in $(0,T-\tau)$, and, due to the dissipation process ($\mu > 0$, $\sigma > 0$),

the weight function $g(\mathbf{r}, 0)$ in (19) decreases as $T - \tau$ increases. If it is the case then (19) is reduced to

$$J(\phi) = \sum_{i=1}^{N} \int_0^T g(\mathbf{r}_i, t) Q_i(t) dt. \tag{20}$$

Peculiarities of the Dual Estimation. The adjoint estimate (19) is equivalent to direct estimate (18), and on the whole, they complement each other nicely in the air quality monitoring. In a specific situation, one of these formulas may be preferable. It should be noted that the direct estimate (18) utilizes solution $\phi(\mathbf{r}, t)$ to problem (1)-(5), and hence, it is necessary to solve this problem again whenever the number N of sources, their positions $\mathbf{r}_i$ or emission rates $Q_i(t)$ vary. The direct evaluation is convenient if the pollution concentrations are to be estimated in each point, or in many zones of domain D. However, such comprehensive information is rather costly and often unnecessary. Sometimes it is sufficient to obtain estimate (18) just for few ecologically important zones of domain D. In this case, a benefit can be gained from applying the adjoint estimate (19) that uses the solution $g(\mathbf{r}, t)$ of adjoint model (10)-(12). Sometimes the estimate (19) provides an immediate response to a nontrivial problem. In particular, adjoint estimates are essential in solving the problem of control of emission rates. Unlike the problem (1)-(5), the adjoint problem (10)-(12) is independent of the number N of sources, their positions $\mathbf{r}_i$ and emission rates $Q_i(t)$, and hence, its solution can be found for each zone Ω irrespective of concrete values of these parameters.

The adjoint method is particularly efficient when the pollution transport problem is considered with time-independent parameters $\overrightarrow{U}(\mathbf{r})$, $\mu(\mathbf{r})$ and $\sigma(\mathbf{r})$, e.g. with climatic wind (Figure 3 and Figure 4). Then solution $g(\mathbf{r}, t)$ of adjoint problem can be calculated for each zone Ω in advance, and kept in a computer. Besides, the solution $g(\mathbf{r}, t)$, once calculated, can be reused for different parameters N, $\mathbf{r}_i$ and $Q_i(t)$. Also, it is important to note that estimate (20) uses the adjoint solution values $g(\mathbf{r}_i, t)$ only in the points $\mathbf{r}_i$ (positions of sources), and hence, it is not necessary to store in the computer the values of adjoint solution in all grid points.

Sensitivity of Estimations. If the number K of zones $\Omega_k \subset D$ ($k = 1, ..., K$) is much less than number N of pollution sources then adjoint estimates (19) are very useful and efficient in the sensitivity study of concentrations $J_k(\phi)$ to variations in emission rates $Q_i(t)$, positions $\mathbf{r}_i$ and number N of sources, and initial pollutant distribution $\phi^0(\mathbf{r})$.

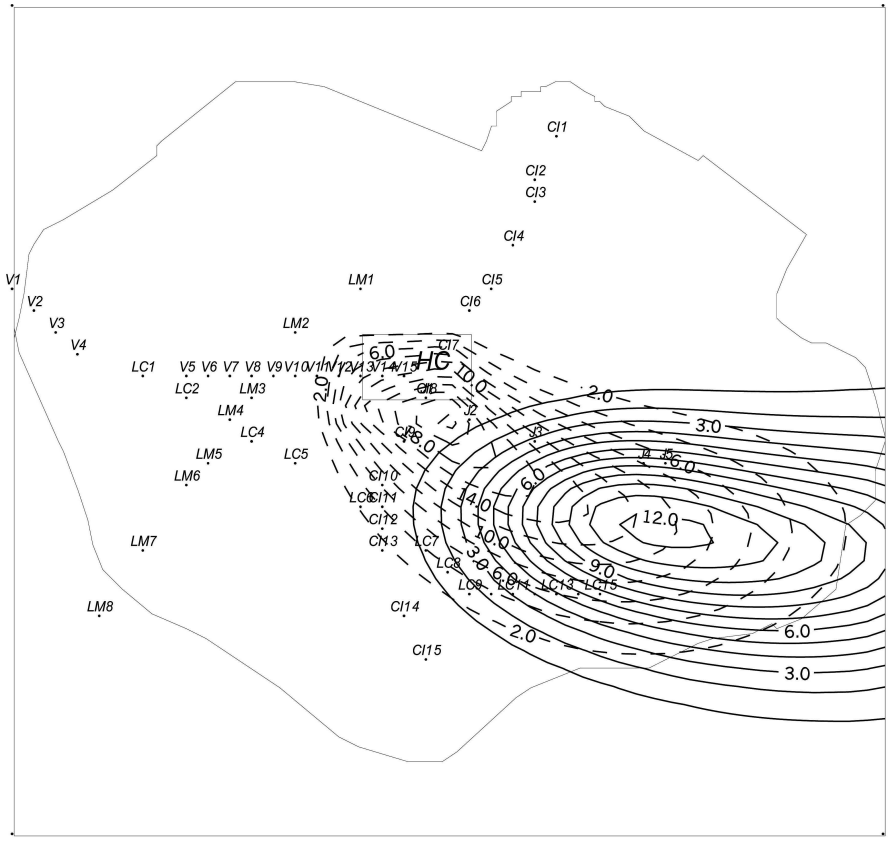

Figure 4: Isolines of solution $g(\mathbf{r}, t)$ calculated at $t = T - 60$ *min* (dotted lines) and $t = T - 90$ *min* (continuous lines); $T = 360$ *min*; Ω is the Colomos park in Guadalajara City.

We derive some sensitivity formulas. Since the problem (1)-(5) is linear, it is easy to get

$$\delta J(\phi) = \sum_{i=1}^{N} \int_0^T g(\mathbf{r}_i, t)\delta Q_i(t)dt + \int_D g(\mathbf{r}, 0)\delta\phi^0(\mathbf{r})d\mathbf{r}, \tag{21}$$

where $\delta J(\phi)$ is a variation in the mean concentration (19) in zone Ω due to variations in $\phi^0(\mathbf{r})$, $Q_i(t)$ and N.

Let us denote by $\mathbf{r}_i$ and $\mathbf{r}_i'$ two different positions of the sources in domain

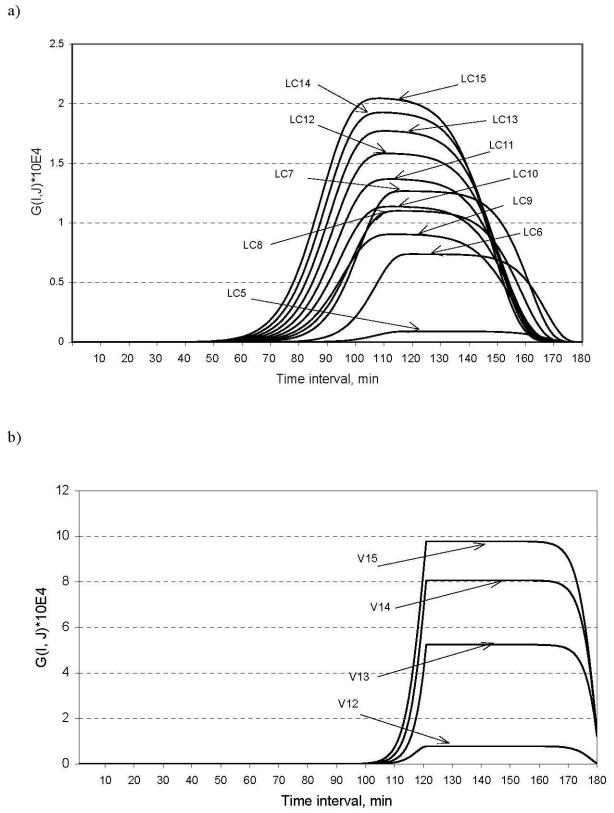

Figure 5: Temporal behavior of adjoint solutions calculated with climatic winds of rainy season for Historical Center of Guadalajara City. The sources are points of the roads: Lazaro Cardenas (a) and Avenida Vallarta (b); $\tau = 60\,min$, $T = 180 min$.

D. Then the $\mathbf{r}_i$-dependence of average concentration $J(\phi)$ can be expressed as

$$\delta J(\phi) = \sum_{i=1}^{N} \int_0^T [g(\mathbf{r}_i', t) - g(\mathbf{r}_i, t)] Q_i(t) dt \tag{22}$$

Note that in (21) and (22) all the variations are arbitrary. Finally, we derive a general formula that can be useful for analyzing the sensitivity of $J(\phi)$ with respect to small variations (errors) in the model parameters. Let ϕ be a solution of problem (1)-(5), and let $\widetilde{\phi} = \phi + \phi'$ be a solution of the perturbed problem

$$\frac{\partial}{\partial t}\widetilde{\phi} + (\overrightarrow{U} + \overrightarrow{U'}) \cdot \nabla\widetilde{\phi} + (\sigma + \sigma')\widetilde{\phi} - \nabla \cdot [(\mu + \mu')\nabla\widetilde{\phi}] = f(\mathbf{r}, t) + f\,'(\mathbf{r}, t) \tag{23}$$

$$\widetilde{\phi}(\mathbf{r},0)=\phi^0(\mathbf{r})+\delta\phi^0(\mathbf{r}) \quad \text{in } D \tag{24}$$

$$\mu\nabla\widetilde{\phi}\cdot\overrightarrow{n}-U_n\widetilde{\phi}=0 \quad \text{at} \quad S^- \quad , \qquad \mu\nabla\widetilde{\phi}\cdot\overrightarrow{n}=0 \quad \text{at} \quad S^+ \tag{25}$$

where

$$f\,'(\mathbf{r},t)=\sum_{i=1}^{N}\delta Q_i(t)\delta(\mathbf{r}-\mathbf{r}_i)\ +\sum_{i=1}^{N}Q_i(t)\delta(\mathbf{r}-[\mathbf{r}_i+\delta\mathbf{r}_i]). \tag{26}$$

For simplicity, we suppose that $\overrightarrow{U'}$ and μ' are reduced to zero at the boundary S. If all the perturbations $\overrightarrow{U'}$, ϕ', μ', σ', $\delta\phi^0$ and $\delta\mathbf{r}_i$ are rather small, the adjoint method as applied to the linearized equation

$$\frac{\partial}{\partial t}\phi'+\overrightarrow{U}\cdot\nabla\phi'+\sigma\phi'-\nabla\cdot(\mu\nabla\phi')=f\,'-\overrightarrow{U'}\cdot\nabla\phi-\sigma'\phi+\nabla\cdot(\mu'\nabla\phi)$$

for perturbations ϕ' gives

$$\begin{aligned}\delta J(\phi)=&\sum_{i=1}^{N}\int_0^T g(\mathbf{r}_i,t)\delta Q_i(t)dt+\int_D g(\mathbf{r},0)\delta\phi^0(\mathbf{r})d\mathbf{r}\\&+\sum_{i=1}^{N}\int_0^T[\nabla g(\mathbf{r}_i,t)\cdot\overrightarrow{\delta\mathbf{r}_i}]Q_i(t)dt\\&-\int_0^T\int_D g[\overrightarrow{U'}\cdot\nabla\phi+\sigma'\phi-\nabla\cdot(\mu'\nabla\phi)]d\mathbf{r}dt.\end{aligned} \tag{27}$$

The first two terms in the right hand side of (27) coincide with (21), while the rest terms show the contribution of small perturbations $\overrightarrow{U'}$, μ', σ' and $\delta\mathbf{r}_i$ to variation in $J(\phi)$ in the zone Ω. Besides, unlike formulas (21) and (22), the last term in (27) already uses the solution $\phi(\mathbf{r},t)$ of non-perturbed problem (1)-(5) in domain $D\times(0,T)$. However, if $\overrightarrow{U'}=\mu'=\sigma'=0$ in D then solution $\phi(\mathbf{r},t)$ is not used, and the adjoint problem (10)-(12) is the only one that must be solved.

4. Simple Examples of Control of Emission Rates

We now pose a problem of the control of emission rates. Let $\mathcal{M}$ be a model (for example the model (1)-(5)) for forecasting the transport and dispersion of a pollutant ϕ in a limited domain $D\subset\mathbb{R}^m$ $(m=2,3)$ and finite time interval $(0,T)$:

$$\mathcal{M}:\ \overrightarrow{Q}(t)\longmapsto\phi\ , \quad \overrightarrow{Q}(t)=(Q_1(t),Q_2(t),...,Q_N(t)),$$

where $Q_i(t)$ is the rate of emission of contaminant ϕ from the ith source located in point $\mathbf{r}_i \in D$ $(i = 1, 2, ..., N)$. The mean concentration of ϕ in a zone $\Omega \subset D$ and time interval $(T - \tau, T)$ is defined by functional (18). If the prediction made with the model $\mathcal{M}$ is unfavorable: $J(\phi_{\overrightarrow{Q}}) > J_0$, where J_0 is the sanitary norm for the pollutant ϕ, then the emission rates $Q_i(t)$ are excessive, and the control problem consists in determining such new (reduced) rates $\overrightarrow{Q^*}(t) = (Q_1^*(t), Q_2^*(t), ..., Q_N^*(t))$, which will lead to the satisfactory result: $J(\phi_{\overrightarrow{Q^*}}) \leq J_0$.

In general, this inverse problem is ill-posed, and hence, it can have many solutions or none, depending on the initial distribution of pollutant $\phi^0(\mathbf{r})$ [43, 44]. To get a well-posed problem, one needs to apply a regularization method that in a sense represents a control strategy. Let us consider three simple examples.

Strategy 1. Control of the Mass of Emitted Contaminant. The first control strategy is defined as the following optimization problem:

$$\min F(\overrightarrow{Q}) = \sum_{i=1}^{N} \|Q_i(t)\|^2 \ , \ \text{subject to } J(\phi_{\overrightarrow{Q}}) \leq J_0, \tag{28}$$

where

$$\|Q_i(t)\| = \sqrt{\int_0^T Q_i^2(t)dt}$$

is the norm in the Hilbert space $L_2(0, T)$. The functional $F(\overrightarrow{Q})$ measures the total mass of pollutant ϕ emitted during time interval $(0, T)$ by N industrial sources located at points $\mathbf{r}_i$ with emission rates $Q_i(t)$. The solution of (28) is

$$Q_i^*(t) = \gamma_i \alpha \frac{g(\mathbf{r}_i, t)}{\|g(\mathbf{r}_i, t)\|^2} \ , \quad i = 1, 2, ..., N, \tag{29}$$

(see [41]), where

$$\alpha = J_0 - \int_D g(\mathbf{r}, 0)\phi^0(\mathbf{r})d\mathbf{r}, \tag{30}$$

$\gamma_1 + \gamma_2 + ... + \gamma_N = 1$ and $\gamma_i = m_i/(\Sigma_{j=1}^N m_j)$ represents the fraction of the total mass of pollutant, emitted by the ith industrial source $(i = 1, 2, ..., N)$ when it works without restricting its capacity [40].

Strategy 2: Control of Temporal Structure of $Q_i(t)$. The control strategy (29), however, has a drawback as it may require a stoppage of sources

for some time, since the intensity of emissions is established proportionally to the values of adjoint function $g(\mathbf{r}_i, t)$ which can be zero. We now formulate a new strategy of control, which restricts the structure of emission rates in $(0, T)$ and does not require stopping the activities of the sources when the adjoint solution $g(\mathbf{r}_i, t)$ vanishes.

The objective is to find such $Q_i^*(t)$ that $J(\phi) \leq J_0$. The idea is that the intensity $Q_i^*(t)$ of ith source may be high while $g(\mathbf{r}_i, t)$ is small, and $Q_i^*(t)$ must be low while $g(\mathbf{r}_i, t)$ is large. The advantage of this approach is that in some time intervals, the ith source would be allowed to operate in full capacity (for example, when $g(\mathbf{r}_i, t) = 0$) [40, 41, 43].

For each i $(i = 1, 2, ..., N)$, we define auxiliary functions

$$G_i(t) = \begin{cases} \alpha[|I_i|\, g(\mathbf{r}_i, t)]^{-1}\ , & \text{if } t \in I_i \\ \delta_i & \text{if } t \in [0, T] \setminus I_i \end{cases}\ , \tag{31}$$

where $I_i = \{t \in [0, T] \mid g(\mathbf{r}_i, t) > 0\}$ and $|I_i|$ denotes its longitude, δ_i is the maximum emission rate corresponding to the ith source, and $[0, T] \setminus I_i$ is the complement of set I_i to set $[0, T]$. The solution is

$$Q_i^*(t) \leq \gamma_i \min\{\delta_i, G_i(t)\} \quad \text{for each } t \in [0, T] \text{ and } i = 1, 2, ..., N. \tag{32}$$

Strategy 3. Optimal Invariant Emission Rates. Let δ_i be the maximum possible emission rate of ith industrial source located at $\mathbf{r}_i$ and

$$a_i = \int_0^T g(\mathbf{r}_i, t)dt > 0$$

$(i = 1, 2, ..., N)$. If $J(\phi) > J_0$ when all plants operate at full power (due to (19) and (30), this means that $\alpha < \Sigma_{i=1}^N a_i \delta_i$) then it is necessary to reduce emission rates. Let us find the maximum possible invariant emission rates $Q_i^* \leq \delta_i$ which minimize the values $\delta_i - Q_i$ and result in $J(\phi) = J_0$, that is,

$$\sum_{i=1}^N a_i Q_i = \alpha.$$

This strategy can be reformulated as the optimization problem

$$\min F(\overrightarrow{Q}) = \sum_{i=1}^N \frac{1}{\gamma_i}[Q_i - \delta_i]^2\ ,\ \text{subject to } \sum_{i=1}^N a_i Q_i = \alpha. \tag{33}$$

Using Lagrange multipliers we obtain

$$\lambda = 2\left(\alpha - \sum_{i=1}^{N} a_i\delta_i\right) / \left(\sum_{i=1}^{N} a_i^2\gamma_i\right),$$

$$Q_i = \delta_i + 0.5\lambda a_i\gamma_i \ , \quad i = 1, 2, ..., N, \tag{34}$$

see [40, 41]. Obviously, $Q_i \leq \delta_i$ for all i, since $\lambda < 0$, and $Q_i \approx \delta_i$ for small γ_i. Thus, this control mainly limits emissions of the powerful industrial plants, for which the corresponding values a_i are not small.

5. General Optimal Control Strategy

Let

$$F(\overrightarrow{Q}) = \left\|\overrightarrow{Q} - \overrightarrow{q}\right\|^2 = \sum_{i=1}^{N} \|Q_i - q_i\|^2_{L_2(0,T)} = \sum_{i=1}^{N} \int_0^T (Q_i - q_i)^2 dt \tag{35}$$

be a functional defined in the domain

$$\Theta = \left\{ q_i(t) \in L_2(0,T); \quad q_i(t) \geq 0 \ , \quad i = 1, 2, ..., N \quad \middle| \ J(\phi_{\overrightarrow{q}}) \leq J_0 \right\} \tag{36}$$

of emission rates $\overrightarrow{q}$ which guarantee the compliance with the sanitary standard in zone Ω: $J(\phi_{\overrightarrow{q}}) \leq J_0$. The optimal control problem consists in finding such $\overrightarrow{Q^*}(t) \in \Theta$ that

$$F(\overrightarrow{Q^*}) = \inf_{\overrightarrow{q} \in \mathcal{Q}} F(\overrightarrow{q}), \tag{37}$$

see [40, 41]. Evidently, the control depends on the norm $\|\cdot\|$ used, and solution $\overrightarrow{Q^*}(t)$ represents the least restriction imposed by the control on the sources. Such variational problem is usually solved with an iterative optimization method, which applies successive evaluation of the dynamic model $\mathcal{M}$ [13, 52]. In general, this process is not very efficient since requires a lot of computations due to the complexity of model $\mathcal{M}$. We now describe a method based on the use of adjoint operator, which allows solving the optimal control problem without consistent estimation of model $\mathcal{M}$.

It should be noted that the solution of problem (37) depends crucially on the parameter α defined by (30). If $\alpha < 0$ then, there is no solution to problem (37) because the health standard is violated even if all the emission rates are

reduced to zero (that is, any industrial activity is stopped). The following three assertions of this section were proved in [44, 45].

Theorem 1. *If* $\alpha = 0$, *then the only solution of optimal control problem (37) is*

$$Q_i^*(t) = \begin{cases} 0\ , & \text{if } t \in I_i \\ Q_i(t) & \text{if } t \in [0,T] \setminus I_i \end{cases},$$

where $I_i = \{t \in [0,T] \mid g(\mathbf{r}_i, t) > 0\}$.

Theorem 2. *Let* $\alpha > 0$. *Then the optimal control problem (37) has unique solution* $\vec{Q}^* \in \Theta$, *besides,* $Q_i^*(t) \leq Q_i(t)$ $(t \in (0,T), \quad i = 1,2,...,N)$ *and* $J(\phi_{\overrightarrow{Q^*}}) = J_0$.

In the case of only one source, the formulation of Theorem 2 can be specified, as follows.

Theorem 3. *Let* $Q(t)$ *be an emission rate of the single point source located at* $\mathbf{r}_0$, *and* $J(\phi_{\overrightarrow{Q}}) > J_0$. *Then*

$$Q^*(t) = Q(t) - \beta g(\mathbf{r}_0, t)\ , \quad \beta = [J(\phi_Q) - J_0]\ /\ \int_0^T g^2(\mathbf{r}_0, t)dt \tag{38}$$

is the solution of optimal control problem (37), provided that it is a non-negative function in $[0,T]$.

Due to Theorem 2, the feasibility set (36) is reduced to

$$\Theta = \left\{ \begin{array}{c} q_i(t) \in L_2(0,T); \\ q_i(t) \geq 0\ , \quad i = 1,2,...,N \end{array} \quad \middle| \quad \sum_{i=1}^{N} \int_0^T g(\mathbf{r}_i, t) q_i(t) dt = \alpha \right\}. \tag{39}$$

An approximate (numerical) solution to the optimal control problem can be obtained with rather effective numerical algorithm of successive orthogonal projections [44]. From computational point of view, the new feasibility set (39) has a considerable advantage over the set (36).

Control by Convex Lineal Combinations. One can develop a new strategy to control using a convex linear combination of the existing ones. Let $\xi_1, \xi_2, ..., \xi_K$ be nonnegative constants such that $\xi_1 + \xi_2 + ... + \xi_K = 1$, where K is the number of control strategies previously defined, besides, each strategy ensures compliance with the health standard in the zone Ω: $J(\phi) \leq J_0$. Let

$Q^*_{ik}(t)$ be the emission rate corresponding to the ith source defined by means of the kth control strategy. Then the emission rates

$$q^*_i(t) = \sum_{k=1}^{K} \xi_k Q^*_{ik}(t) \ , \quad i = 1, 2, ..., N \tag{40}$$

represent a new sufficient (non-optimal) strategy that also guarantees compliance with the health standard in the zone $\Omega : J(\phi) \leq J_0$.

6. Two Examples of Application of Control Strategies

Example 1. Let us consider a square domain $D = (0, 2km) \times (0, 2km)$ with a single point source located at $\mathbf{r}_0 = (1.8, 0.2)$ which emits lead particles with emission rate $Q = 3.8\ kg/h$. For simplicity, the initial lead distribution is disregarded, $\phi^0(\mathbf{r}) = 0$ in D. The deposition and diffusion coefficients are $\sigma = 0.001\ h^{-1}$ and $\mu = 0.04\ km^2/h$. The non-divergent wind velocity $\overrightarrow{U}(\mathbf{r}) = \{u(\mathbf{r}), v(\mathbf{r})\}$ is defined by the stream function $\Psi = xy$:

$$u = -\Psi_y = -x \ , \quad v = \Psi_x = y.$$

The dispersion model (1)-(5) and its adjoint (10)-(12) are considered in the four-hour interval $(0, T)$. We will monitor the mean lead concentration $J(\phi)$ in zone $\Omega = [0, 0.5] \times [0.5, 1.0]$ during the same time period ($\tau = T = 4\ h$). The sanitary norm is $J_0 = 1.5\ \mu g/m^3$ [55].

Figure 6 shows the contour levels of lead each hour, and one can see a clear increase of lead in changing the direction of wind from south-east to north-west. Figure 7 shows the isolines of solution $g(\mathbf{r}, t)$ of adjoint model (10)-(12), and one can observe that during four hours (from $t = 4$ to $t = 0$), the step function $p(\mathbf{r}, t)$ shifts in the direction of vector $-\overrightarrow{U}$ (that is, from north-west to south-east), as it should. The mean lead concentration $J(\phi)$ calculated in zone Ω with emission rate Q is $2.11\ \mu g/m^3$. Since the result is unsatisfactory (the sanitary norm J_0 is exceeded), we apply and compare five different control strategies: the control strategies (29), (32) and (34) with emission rates $Q_i \equiv Q^*_i$ $(i = 1, 2, 3)$ and two control strategies defined with the convex linear combinations $Q_4 = 0.3 \cdot Q_1 + 0.7 \cdot Q_3$ and $Q_5 = 0.5 \cdot Q_2 + 0.5 \cdot Q_3$.

The mean lead concentrations obtained in zone Ω when the model (1)-(5) is solved with emission rates $Q^*_i(t)$, prescribed by the five control strategies $(i = 1, ..., 5)$, are shown in Table 1, while Figure 8 shows the temporal behavior of $Q_i(t)$.

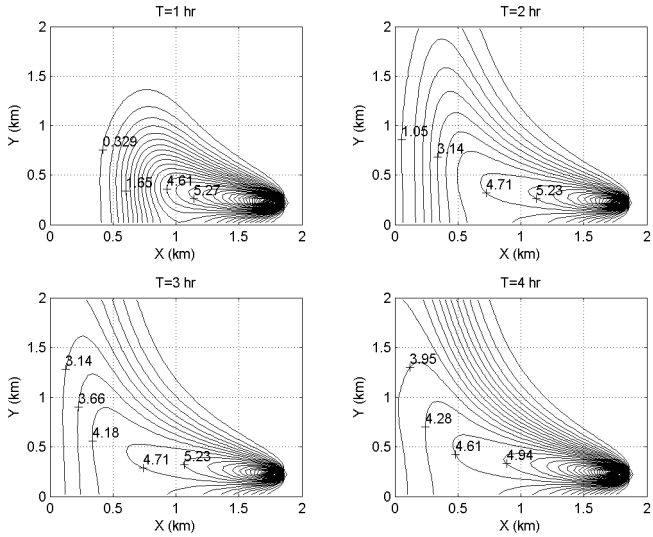

Figure 6: Isolines of the lead concentration $\phi(\mathbf{r}, t)$ calculated for $t = 1$ *hour*, $t = 2$ *hours*, $t = 3$ *hours* and $t = 4$ *hours*.

k	$c1$	$c2$	$c3$
1	0.8	0.8	0.8
2	1.0	0.8	0.5
3	0.5	1.0	1.5
4	1.2	0.5	1.2
5	0.6	1.2	0.6
6	0.6	0.6	1.5
7	1.5	0.6	0.6

Table 1: Mean lead concentrations $J(\phi)$ in Ω.

Each of the five management strategies meets the standard of health and provides an alternative to the original source intensity Q, however, the rates Q_3 (optimal control) and also Q_4 and Q_5 (convex control) are most preferred because they require less radical changes in the intensity of the original source. Although the emission rate Q_2 is only 40% of original rate Q in the first half of the time, it coincides with the original rate Q during the second half of the

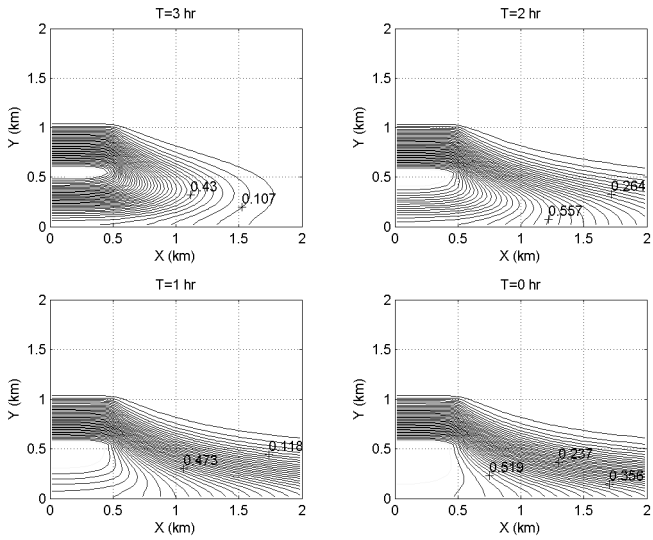

Figure 7: Isolines of the solution of adjoint model $g(\mathbf{r}, t)$ for $t = 3$ *hours*, $t = 2$ *hours*, $t = 1$ *hour* and $t = 0$.

time, and this fact can also be attractive.

Also, like the original rate Q, the optimal emission rate Q_3 is stationary and represents 71% of Q. This makes Q_3 a simple alternative to the original industrial source activity. Finally, among the five strategies, the first strategy with emission rate Q_1 has the most serious consequences for the industrial plant activity, because it requires the work stoppage for 25% of the total time.

Example 2. Suppose that all data are the same as in Example 1, but we now consider four different original emission rates of the source located at $\mathbf{r}_0 = (1.8, 0.2)$:

$$Q_1(t) = 3.8\ , \quad Q_2(t) = \begin{cases} 4\ , & \text{if } 0 \le t < 1 \\ 5 - t & \text{if } 1 \le t \le 4 \end{cases}$$

$$Q_3(t) = \cos \pi t + 3.5\ , \quad Q_4(t) = \begin{cases} 3\ , & \text{if } 0 \le t < 1 \\ \frac{2}{3}(t-1) + 3 & \text{if } 1 \le t \le 4 \end{cases}$$

Thus, Q_1 is constant, Q_2 is invariable during the first hour and then linearly decreases, Q_3 is a periodic function with the period of two hours, and Q_4 is invariable during the first hour and then linearly increases. The mean lead

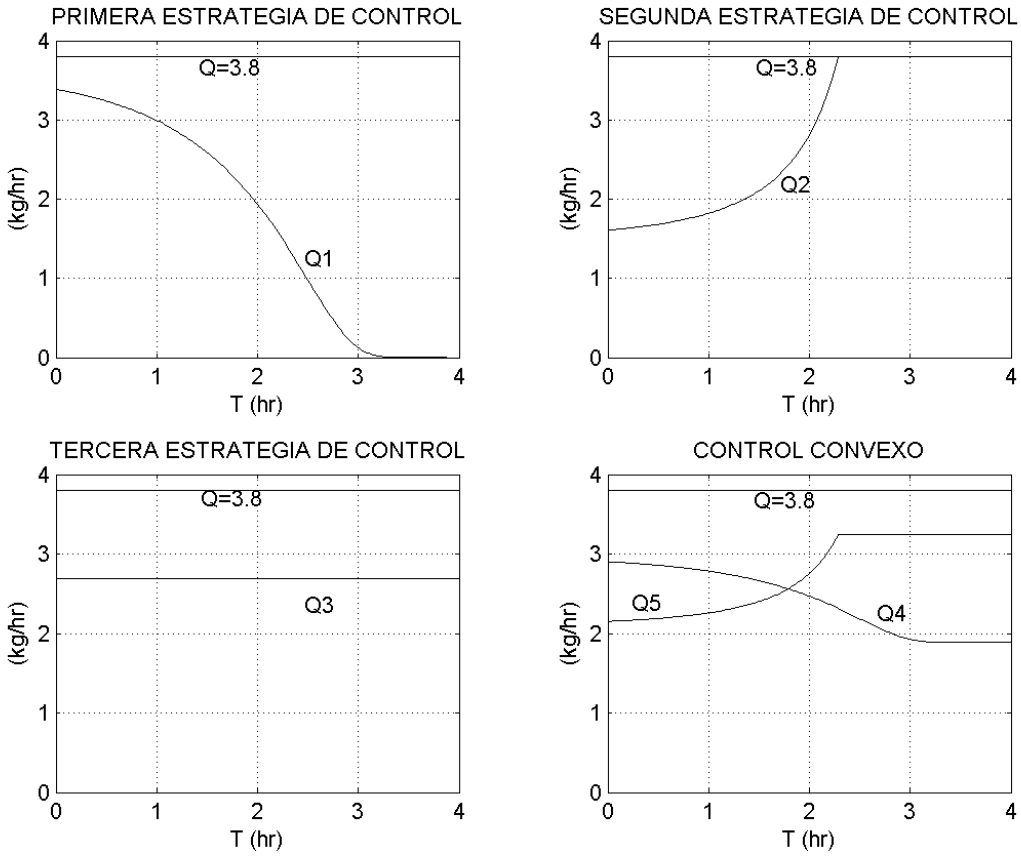

Figure 8: Emission rates obtained with five control strategies.

concentrations $J(\phi)$ calculated in zone Ω with each emission rate Q_i $(i = 1, ..., 4)$ are 2.11 $\mu g/m^3$, 2.02 $\mu g/m^3$, 1.97 $\mu g/m^3$ and 1.81 $\mu g/m^3$, respectively. Since all the results are unsatisfactory (each one exceeds the sanitary norm $J_0 = 1.5$ $\mu g/m^3$), we apply the optimal control method (38). The original emission rates $Q_i(t)$ and optimal emission rates $q_{\text{opt}i}(t)$ given by the control are shown in Figure 9. In all four cases, the mean lead concentrations $J(\phi)$ obtained with the optimal emission rates $q_{\text{opt}i}(t)$ coincide with the sanitary norm J_0, as they should.

In full agreement with the theory $q_{\text{opt}i}(t) \leq Q_i(t)$ for all $t \in (0, 4)$ and $1 \leq i \leq 4$, also Figure 9 shows that for each i, $q_{\text{opt}i}(t) = Q_i(t)$ during the last

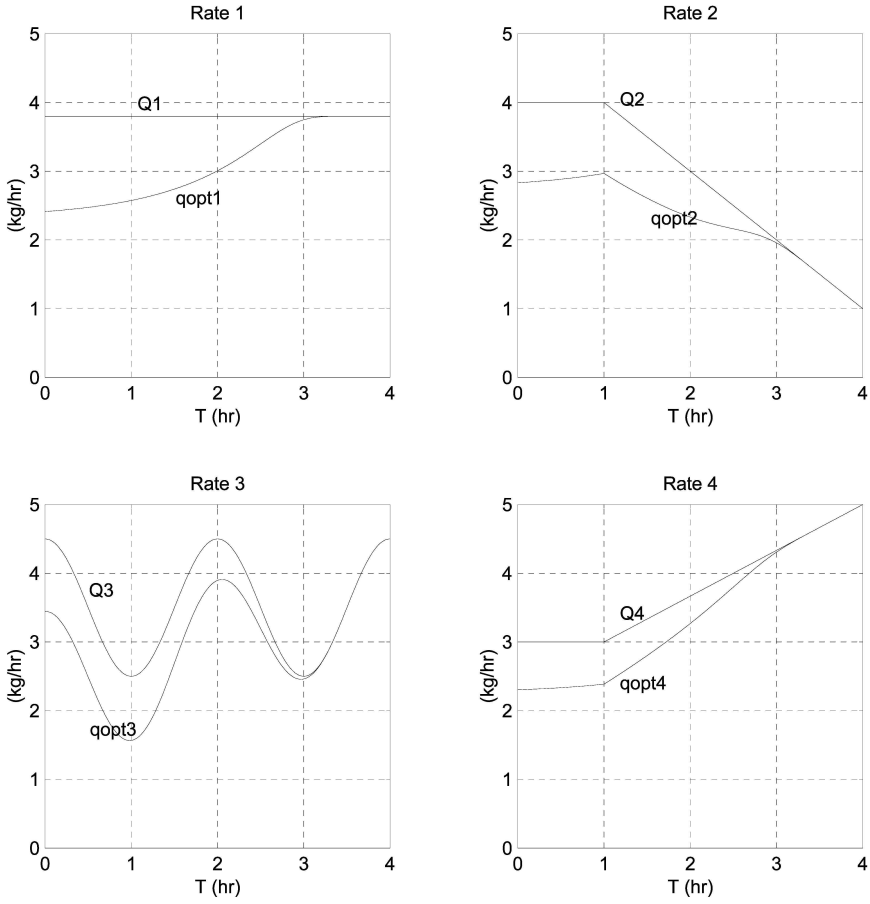

Figure 9: Temporal behavior of original emission rates $Q_i(t)$ and optimal emission rates $q_{\mathrm{opt}i}(t)$ in four experiments.

hour ($3 \leq t \leq 4$), that is, the emission rates, both optimal and original, coincide with each other during the entire period of time in which the solution of adjoint model $g(\mathbf{r}_1, t)$ is equal to zero, and hence, the source emissions do not give any contribution to the pollution of zone Ω. Finally, it is interesting to note that in the interval $0 \leq t < 3$, in which these values do not match, the temporal behavior of each optimal emission rate $q_{\mathrm{opt}i}(t)$ is similar to the corresponding original rate $Q_i(t)$. This result is something useful for the industry as the

optimal strategy (38) does not require a radical change in the mode of its operation.

7. Remediation of Contaminated Aquatic Systems

It is often necessary to take certain measures to clean aquatic zones, contaminated with biofilm (remediation) or oil (bioremediation). We now apply the optimal control strategy to this problem. Suppose that we must purify N polluted zones Ω_i in an aquatic system by using a chemical agent (the cleaner), $i = 1, ..., N$, see [45].

Being released at a point $\mathbf{r}_0 \in D$, the chemical agent spreads due to advection and diffusion, and while reaching the zones Ω_i, purifies polluted water. Our aim is to find such optimal point $\mathbf{r}_0$ for the release of a chemical substance, which on the one side will result in its minimum consumption, and on the other hand, will generate the minimum concentrations of this substance in the zones Ω_i which are still enough for water purification. Sometimes, when the contaminant is fairly stable (biofilm), the critical concentration c_i of an antimicrobial agent (chlorine, iodine, etc.) must be maintained in each zone Ω_i for a long time interval $(T - \tau, T)$.

Therefore, we need to determine the discharge point $\mathbf{r}_0$ and the emission rate Q which meet the following constraints:

$$J_i(\phi) = c_i \ , \quad i = 1, ..., N, \tag{41}$$

where $\phi(\mathbf{r}, t)$ is the concentration of chemical agent determined by the model (1)-(5) with initial condition $\phi^0(\mathbf{r}) = 0$, and $J_i(\phi)$ is its mean concentration (18) in Ω_i. Furthermore, not to damage the ecology of the environment, the total mass $F(Q)$ of the cleaner discharged into the system should be minimized. Therefore, the optimal control problem is set as follows:

$$\text{minimize } F(Q) = \sqrt{\int_0^T Q^2(t)dt}$$
$$\text{subject to: } \ J_i(\phi) = c_i \ , \quad i = 1, ..., N \ , \ Q \geq 0 \ , \ 0 \leq t \leq T.$$

The analytical and numerical solution of this problem is given in [46]:

$$Q^*(t) = \sum_{i=1}^{N} \frac{\det(\Psi_i)}{\det(\Psi)} g_i(\mathbf{r}_0, t), \qquad \Psi_i = \begin{pmatrix} \psi_{11} & ... \ c_1 & ... & \psi_{1N} \\ \psi_{21} & ... \ c_2 & ... & \psi_{2N} \\ \vdots & \vdots & \vdots & \vdots \\ \psi_{N1} & ... \ c_N & ... & \psi_{NN} \end{pmatrix}, \tag{42}$$

where $\Psi = \{\psi_{ij}\}$ is the Gram matrix of order N whose entries

$$\psi_{ij} = \int_0^T g_i(\mathbf{r}_0, t) g_j(\mathbf{r}_0, t) dt, \quad 1 \le i, j \le N \tag{43}$$

are the inner products in $L_2(0, T)$ of adjoint functions, and matrix Ψ_j is obtained from Ψ by replacing its ith column with the corresponding components of the vector of critical concentrations $\overrightarrow{c} = (c_1, \ldots, c_N)^T$. It is easily seen from (43) that matrix Ψ is symmetric. Moreover, Ψ is also a positive semidefinite matrix, since

$$\overrightarrow{x}^t \Psi \overrightarrow{x} = \left\| \sum_{i=1}^N x_i g_i(\mathbf{r}_0, t) \right\|^2 \ge 0.$$

In the case when the adjoint functions $\{g_i(\mathbf{r}_0, t)\}_{i=1}^N$ are linearly independent, matrix Ψ is positive definite, and hence, non-singular, and the optimal discharge rate Q^* is well defined by (42).

The optimal discharge point $\mathbf{r}_0$ is obtained while minimizing the functional

$$\|Q^*\|^2 = \frac{1}{\det(\Psi(\mathbf{r}_0))} \sum_{i=1}^N c_i \ \det(\Psi_i(\mathbf{r}_0)).$$

Example 3. In order to illustrate the method we now consider a simple example of remediation in a three-dimensional channel of one hundred and twenty meters long $[0, 120]$, ten meters wide $[0, 10]$, and four meters deep $[0, 4]$. We consider in the channel three zones Ω_i contaminated by biofilms ($N = 3$): $\Omega_1 = [20, 30] \times [9, 10] \times [0.4]$, $\Omega_2 = [70, 80] \times [9, 10] \times [0.4]$ and $\Omega_3 = [95, 100] \times [0, 2] \times [0.4]$.

The critical concentrations of the cleaner c_i (gr/m^3) in the zones vary from one experiment to another (Table 2) and generate different optimal discharge rates Q_k^* (Figure 11). The parameters of three-dimensional adjoint model (10)-(12) have been taken as follow: the velocity vector $\overrightarrow{U}$ is directed along the channel and is equal to 30 m/h, $\mu = 6$ m^2/h, $\sigma = 1$ h^{-1}, and the processes of evaporation and sedimentation are ignored here. The cleaner (chlorine) is discharged at the point $\mathbf{r}_0 = (3, 2.2, 2)$ during the total time interval of 4 hours: $(0, T) \equiv (0, 4)$, and the mean concentration is controlled within the last one-hour interval $(3, 4)$, i.e., $\tau = 1$ h.

Adjoint functions $g_i(\mathbf{r}_0, t)$ for the three zones ($i = 1, 2, 3$) are given in Figure 10, while optimal discharge rates are shown in Figure 11. For the 7th experiment, evolution of the mean chlorine concentration in the zones Ω_i $(i = 1, 2, 3)$

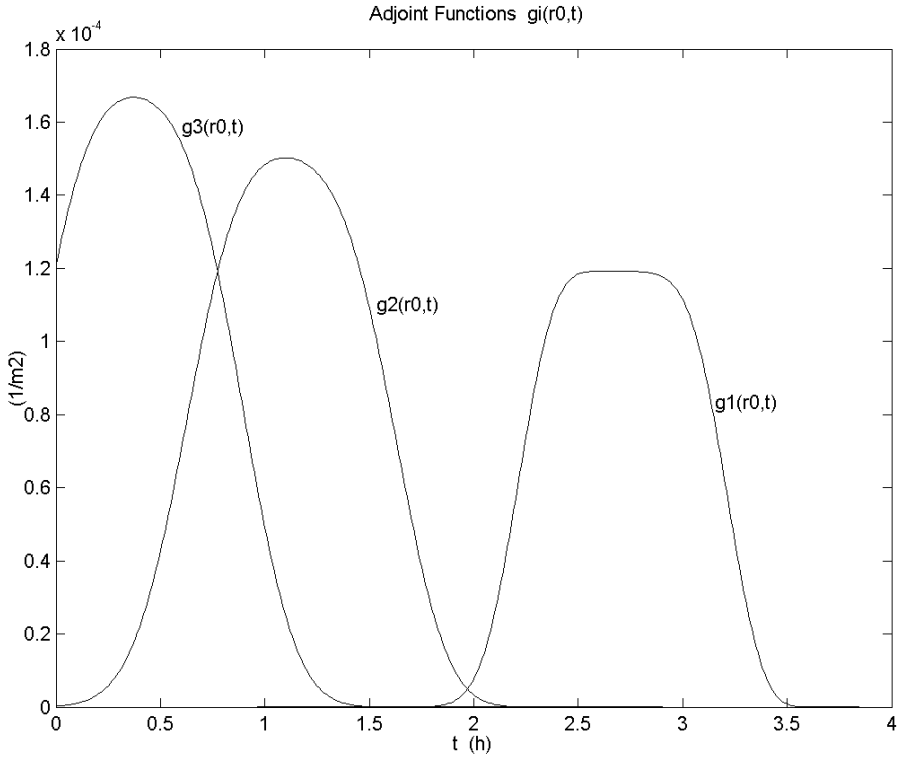

Figure 10: Adjoint functions $g_i(\mathbf{r}_0, t)$, $i = 1, 2, 3$.

Tasa de emisión	$J(\phi)$ $\left(\mu g / m^3\right)$
Q	2.11
Q_1^*	1.50
Q_2^*	1.18
Q_3^*	1.50
$Q_4^* = 0.3 \cdot Q_1^* + 0.7 \cdot Q_3^*$	1.50
$Q_5^* = 0.5 \cdot Q_2^* + 0.5 \cdot Q_3^*$	1.34

Table 2: Critical chlorine concentrations in zones Ω_i, $i = 1, 2, 3$.

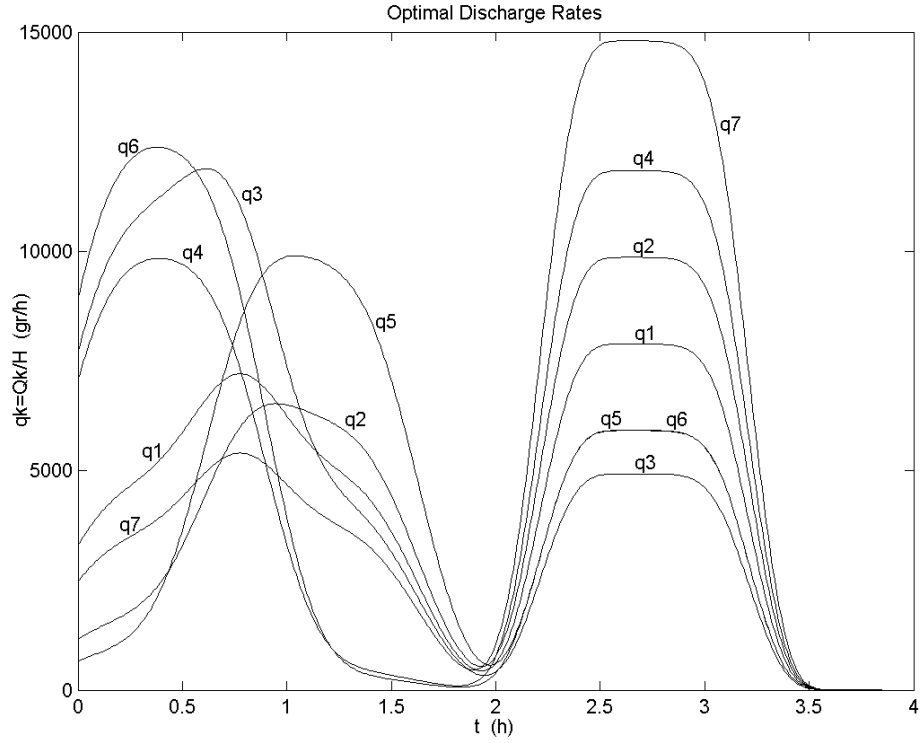

Figure 11: Optimal discharge rates $q_k(t)$, $k = 1, ..., 7$.

is shown in Figure 12, while isolines of the mean chlorine concentration in domain D at the final moment $T = 4h$ are presented in Figure 13. The optimal discharge rate applied is $Q_7(t)$. In every experiment, the optimal discharge rate has successfully been found using equation (42).

8. Conclusions

In this work, we suggest a few methods for estimating the mean concentration of pollutants in ecologically sensitive zones and for preventing their dangerous levels through a control of emission rates of sources. The methods are based on the adjoint approach utilizing dual (direct and adjoint) pollution concentration estimates in a zone. In the adjoint estimates, which depend explicitly on the number, positions and emission rates of the sources and the initial distribution

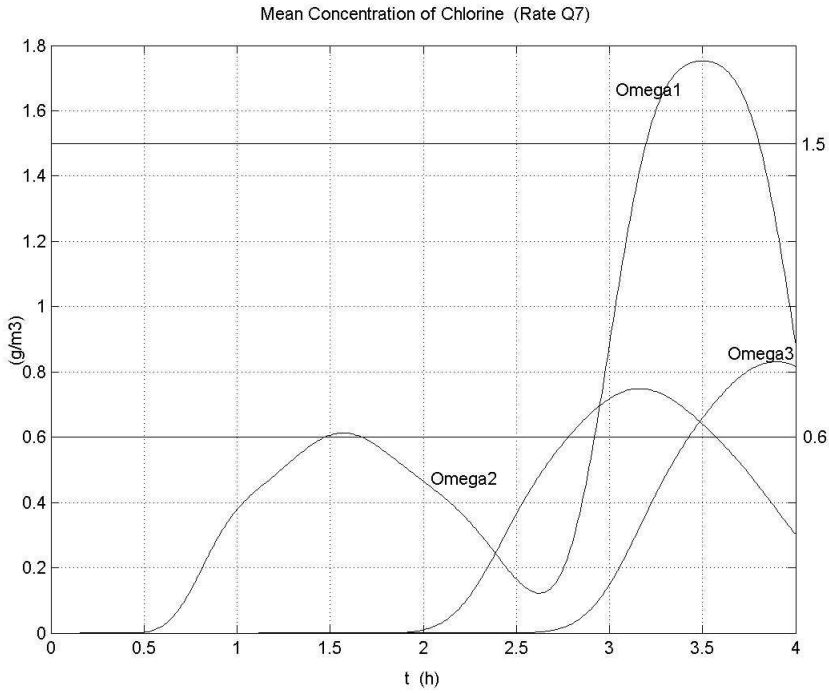

Figure 12: Evolution of mean concentration of cleaner in zones Ω_i, $i = 1, 2, 3$. The optimal discharge rate applied is $Q_7(t)$.

of pollutants in the region, the solutions of adjoint problem serve as weight function providing valuable information on the contribution of each source and initial data to the pollution of the zone. This makes these estimates very efficient in studying the model response to variations in the emission rates and initial conditions, and in developing various control strategies.

Various control strategies, both non-optimal (sufficient) and optimal, have been developed. The objective of each control strategy is to avoid violations of existing sanitary norm through reductions in the emission rates of sources. Such control strategies are designed using the direct and adjoint models of advection and diffusion of pollutants, and taking into account the number of point sources to control, their locations and corresponding sanitary norms. The methods are illustrated by simple examples. It is also shown the application of the optimal control strategy for cleaning aquatic zones contaminated with biofilm (remediation) or oil (bioremediation).

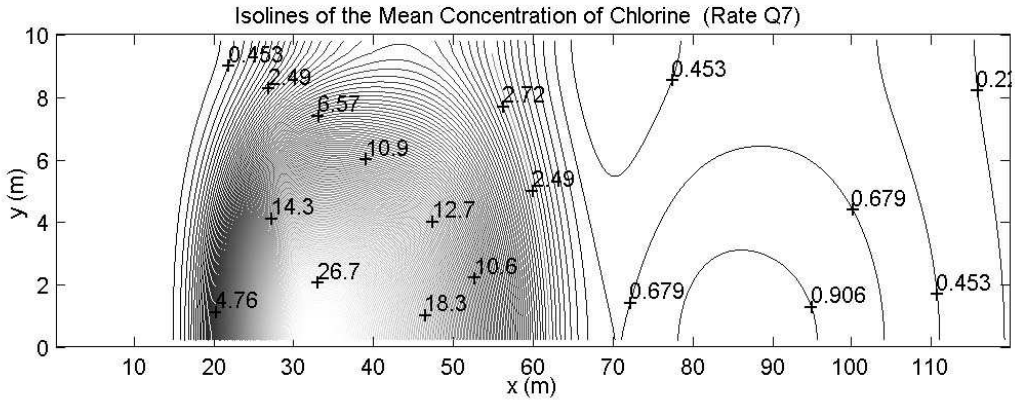

Figure 13: Isolines of mean concentration of nutrient in region D at final moment $T = 4\ hours$. The optimal discharge rate applied is $Q_7(t)$.

Acknowledgments

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