Optimal emission control and identification of an unknown pollution source

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Abstract. The advection-diffusion-reaction equation is used for describing the dispersion of a quasi-passive contaminant from industrial point sources in a limited area. The conditions established on the open boundary ensure that the problem is correct in the sense of Hadamard, that is, its solution exists, is unique, and is stable to initial perturbations. The Lagrange identity is used to construct the adjoint operator and formulate an adjoint problem. Equivalent direct and adjoint estimates are derived to assess the concentration of the pollutant at monitoring sites of the area. Formulas obtained on the basis of adjoint estimates are useful in analyzing the sensitivity of the model to both variations in the intensity of pollution sources and variations in the initial distribution of the pollutant concentration in the area. New optimal emission control strategies based on using the adjoint estimates are developed in order to prevent violations of existing sanitary standards by timely reduction of emission rates of operating sources. Optimal control here lies in minimizing these reductions. In addition, this control is primarily aimed at reducing the intensity of emissions from sources that most pollute the monitoring site. Also, new methods are proposed for identifying the main parameters of an unknown point source that arose as a result of a dangerous incident (accident, explosion, etc.). These methods allow determining the location and intensity of a constant or non-stationary point source, as well as the moment of emission of a pollutant in the case of an instantaneous point source. This helps to quickly assess the scale of the incident and its consequences. Numerical results show the effectiveness of the methods.

1. Introduction

During the last century, anthropogenic activities emit into the atmosphere at short intervals, such large volumes of substances that the mechanisms of assimilation do not have time to recycle the excess chemicals and to clean the atmosphere. A pollutant, depending on its concentration and toxicity, causes various health problems, from respiratory discomfort in healthy people to the increase in mortality among vulnerable populations. Consequently, it is important to design methods for controlling emissions and reducing the concentration of hazardous substances to acceptable health standards.

In this work, simple mathematical models of pollutant dispersion as well as their adjoint models are used to assess pollution levels at the monitoring sites, develop optimal strategies to control emission rates of the point sources and determine the location and intensity of unknown sources of pollution. The emission control strategies are optimal in the sense that they set minimal limits on the rate of emissions from sources to avoid exceeding sanitary standards. Whenever the dispersion model predicts a sanitation violation at the current emission levels, a control (i.e., a restriction of intensity of emissions) can be applied. Thus, mathematical control methods are an effective complement to the use of “green” technologies.

The determination of the intensity and location of unknown sources using the observed data is an inverse
problem that, in the presence of observational errors, requires the use of regularization methods. In the present work, we suggest methods for assessing the main parameters of an unknown point source with stationary, instantaneous and nonstationary emission rate.

2. Air pollution dispersion model in a limited area

Sea $D$ a two-dimensional limited domain with boundary $S$. Suppose there are $N$ industrial point sources located at points $r_i = (x_i, y_i)$ of the domain $D$ ($i = 1, 2, ..., N$). Let $\phi(r, t)$ be the concentration of a pollutant at point $r = (x, y)$ and the moment $t$. To study the propagation of the pollutant, we consider in the domain $D$ and time interval $(0, T)$ a 2D (vertically averaged) pollution dispersion model

$$\phi_t + \text{div}(U \phi) + \sigma \phi - \text{div}(\mu \nabla \phi) = f(r, t)$$

(1)

where $U(r, t) = [u(r, t), v(r, t)]$ is the wind velocity vector (known from observations or some dynamic model), $\sigma(r, t) > 0$ characterizes the rate of exponential decay of $\phi(r, t)$ due to various physical and chemical processes, $\mu(r, t) > 0$ is the turbulent diffusion coefficient,

$$f(r, t) = \sum_{i=1}^{N} Q_i(t) \delta(r - r_i)$$

(2)

$Q_i(t)$ is the emission rate of the $i$-th source, and $\delta(r - r_i)$ is the Dirac function. It is assumed that

$$\text{div } U = 0$$

(3)

Eq. (1) is solved with the initial condition

$$\phi(r, 0) = \phi^0(r) \quad \text{at} \quad t = 0$$

(4)

Normally the pollution flux through the open boundary $S$ of limited area $D$ is unknown. It is therefore important to put such boundary conditions, under which the problem will be posed correctly in a limited area, both physically and mathematically.

For this purpose, we denote by $U_n = U \cdot n$ the projection of velocity $U$ on the unit external normal $n$ to the boundary $S$ of domain $D$, and divide $S$ into the “inflow” part $S^-$ (where $U_n < 0$, and the pollution flux is directed inside $D$) and “outflow” part $S^+$ (where $U_n \geq 0$, and the pollution flux is directed outside $D$) (Fig.1). Then we take the following boundary conditions:

$$\mu \frac{\partial}{\partial n} \phi = 0 \quad \text{at} \quad S^- \quad \text{and} \quad \mu \frac{\partial}{\partial n} \phi - U_n \phi = 0 \quad \text{at} \quad S^+$$

(5)

[3]. It was shown in [8] that problem (1)-(5) is well posed because it has a unique solution that continuously depends on the initial distribution $\phi^0(r)$ and on the number $N$, emission rates $Q_i(t)$ and positions $r_i$ of the sources.

Figure 1. Domain $D$ with open boundary $S = S^- \cup S^+$. 
The solution of problem (1)-(5) satisfies two integral equations

\[
\frac{\partial}{\partial t} \int_{D} \phi \, dr = \sum_{i=1}^{N} Q_i(t) - \int_{D} \sigma \phi \, dr - \int_{S} U_n \phi \, ds
\]  

(6)

\[
\frac{\partial}{\partial t} \int_{D} \phi^2 \, dr = 2 \sum_{i=1}^{N} Q_i(t) \phi(r,t) - 2 \int_{D} (\sigma \phi^2 + \mu |\nabla \phi|^2) \, dr - \int_{S} U_n |\phi|^2 \, ds
\]  

(7)

Thus, the total mass \( \int_{D} \phi \, dr \) and the solution norm \( \|\phi\| = \left( \int_{D} \phi^2 \, dr \right)^{1/2} \) increase if \( Q_i(t) > 0 \) and decrease under influence of dissipation \( \sigma > 0 \), diffusion \( \mu > 0 \), and advective flow of pollution across the boundary \( S \) of domain \( D \). If \( Q_i(t) = 0 \), \( \sigma = 0 \), \( \mu = 0 \) and \( U_n = 0 \) everywhere at the boundary \( S \), then both integrals are invariable in time:

\[
\left. \int_{D} \phi(t,r) \, dr = \text{const} \right\}, \quad \|\phi(t,r)\| = \text{const}
\]  

(8)

Equations (6)-(8) are useful in testing computational programs.

3. Air quality assessment

The solution of dispersion problem (1)-(5) allows one to estimate the concentration of the pollutant in any point or zone of domain \( D \times (0,T) \). However, if one need to answer the question “To what extent each source is responsible for the contamination of a particular zone?” then this method requires solving \( N \) problems (1)-(5) separately with \( f(r,t) = Q_i(t) \delta(r-r_i) \), \( i = 1, 2, \ldots, N \). Therefore, we now describe another approach that makes it easier to answer this question, especially if the number of sources \( N \) is large.

Using the Lagrange identity [2] it is possible to define the operator adjoint to the operator of model (1)-(5) and formulate the adjoint problem in the domain \( D \) and time interval \((0,T)\):

\[
- \frac{\partial g}{\partial t} \cdot \text{div}(Ug) + \sigma g - \text{div}(\mu \nabla g) = p(r,t) \quad \text{in} \ D \times (0,T)
\]  

(9)

\[
g(r,T) = 0 \quad \text{in} \ D
\]  

(10)

\[
\mu \frac{\partial g}{\partial n} + U_n g = 0 \quad \text{at} \ S^+ \quad \text{and} \quad \frac{\partial g}{\partial n} = 0 \quad \text{at} \ S^-
\]  

(11)

The wind velocity \( U(r,t) \) and coefficients \( \mu(r,t) > 0 \) and \( \sigma(r,t) > 0 \) in problem (9)-(11) are the same as in problem (1)-(5). Let us put \( f(r,t) = 0 \) and \( p(r,t) = 0 \), and use the substitution \( t' = T - t \) in Eq. (9). Then one can see that Eq. (9) differs from Eq. (1) only in the sign of the velocity \( U \). As a result, the boundary parts \( S^+ \) and \( S^- \) of problems (1)-(5) and (9)-(11) are swapped. In addition, problem (9)-(11) is well posed only if it is solved in the opposite time direction: from \( t = T \) to \( t = 0 \) [8]. That is why the “initial” condition (10) is posed at the moment \( t = T \).

Denote by \( \phi(r,t) \) the concentration of the pollutant at the point \((r,t)\) of the space-time domain \( D \times (0,T) \). Let \( \Omega \) be a monitoring zone with area \( |\Omega| \) in domain \( D \). Then

\[
J(\phi) = \frac{1}{\tau |\Omega|} \int_{T-\tau}^{T} \int_{\partial D} \phi(r,t) \, dr \, dt
\]  

(12)

is the mean concentration of the pollutant in the monitoring zone \( \Omega \) and time interval \((T-\tau,T)\) where \( 0 \leq \tau \leq T \).

We will now obtain two adjoint estimates of air pollution which are equivalent to the direct estimates (12) and \( \phi(r,t) \). To this end, let us subtract the equation (9) pre-multiplied by \( \phi(r,t) \) from the equation (1) pre-multiplied by \( g(r,t) \), and integrate the result over domain \( D \times (0,T) \). Then conditions (4)-(5) and (10)-(11) lead to
\[
\int_0^T \int_D p(r,t)\phi(r,t)drdt = \sum_{i=1}^{N} \int_0^T g(r_i,t)Q_i(t)dt + \int_D g(r,0)\phi^0(r)dr
\]

If we put
\[
p(r,t) = \begin{cases} 
1/(\tau |Q|), & \text{if } (r,t) \in \Omega \times (T - \tau, T) \\
0, & \text{otherwise}
\end{cases}
\]
in (9) then (13) leads to the first adjoint estimate
\[
J(\phi) = \sum_{i=1}^{N} \int_0^T g(r_i,t)Q_i(t)dt + \int_D g(r,0)\phi^0(r)dr
\]

And putting \( p(r,t) = \delta(r-r_t)\delta(t-t_j) \) in (9) we obtain the second adjoint estimate
\[
\phi(r_j,t_j) = \sum_{i=1}^{N} \int_0^{t_j} g(r_i,t)Q_i(t)dt + \int_D g(r,0)\phi^0(r)dr
\]

where it was taken into account that \( g(r_i,t) = 0 \) in the interval \((t_j, T)\). The advantage of adjoint estimates is that they explicitly depend on the emission rates \( Q_i(t) \) of the sources and initial distribution \( \phi^0(r) \) in \( D \), whose contribution is determined by the values of weight functions \( g(r_i,t) \) and \( g(r,0) \), respectively. Note that the last integrals in estimates (15) and (16) are negligible if the corresponding intervals \((0, T - \tau) \) and \((0, t_j) \) are sufficiently large. Indeed, \( p(r,t) = 0 \) during these intervals, while the dissipation processes \( (\mu > 0, \sigma > 0) \) reduce the values of \( g(r,0) \).

The direct and adjoint estimates complement each other quite well, and in a specific situation one of these estimates may be preferable. The direct estimates \( \phi(r_j,t_j) \) and (12) are useful if the pollution concentration is estimated at many points or zones of domain \( D \). However, problem (1)-(5) must be solved again whenever the number \( N \) of sources, their locations \( r_i \) or emission rates \( Q_i(t) \) change. In contrast to problem (1)-(5), the solution of the adjoint problem (9)-(11) does not depend on the parameters \( N, r_i \) and \( Q_i(t) \). Therefore, if the values of \( \phi(r_j,t_j) \) and \( J(\phi) \) are needed only at a few points or zones of domain \( D \), it is better to solve the adjoint problem (9)-(11) and use the adjoint estimates (15) and (16). Sometimes, the adjoint estimates help to quickly solve non-trivial problems. In addition, these estimates are important for controlling the emission rate of pollution sources and identifying the parameters of an unknown source of pollution.

Here are two formulas useful in studying the sensitivity of estimate (15) (or the sensitivity of the solution to the linear problem (1)-(5)):
\[
\delta J(\phi) = \sum_{i=1}^{N} \int_0^T g(r_i,t)\delta Q_i(t)dt + \int_D g(r,0)\delta \phi^0(r)dr
\]
\[
\delta J(\phi) = \sum_{i=1}^{N} \int_0^T [g(r_i',t) - g(r_i,t)]Q_i(t)dt
\]

where \( \delta J(\phi) \) is a variation in the concentration (15) in zone \( \Omega \) due to arbitrary variations in \( \phi^0(r), Q_i(t) \) and \( N \); while \( r_i \) and \( r_i' \) are different locations of sources in domain \( D \).

4. Optimal control of total emissions

Let us formulate a particular problem of emission intensity control. Suppose that we have a dispersion model \( \mathcal{M} \) (for example, the model (1)-(5)) that predicts the concentration of a pollutant \( \phi \) in a space-time domain \( D \times (0, T) \):

\[
\mathcal{M}: Q \rightarrow \phi, \quad Q(t) = (Q_1(t), Q_2(t), ..., Q_N(t))
\]
where \( Q(t) \geq 0 \) is the emission rate of the \( i \)-th source located at \( r_i \in D \) \((i=1,2,...,N)\). Suppose that a forecast of air quality obtained with the model \( M \) in time interval \((0,T)\) is unfavorable, i.e., \( J(\phi) > J_0 \), where \( J(\phi) \) is the mean concentration \((15)\) in a zone \( \Omega \subset D \) during time interval \([T-t,T]\), and \( J_0 \) is the admissible sanitary norm. Then a control can be applied to establish such reduced emission rates \( Q^*(t) \leq Q(t) \) in \((0,T)\) that the re-forecast with the model \( M \) and new rates \( Q^*(t) \) in time interval \((0,T)\) will give the satisfactory result: \( J(\phi) \leq J_0 \).

Consider a simple air pollution control defined as the optimization problem

\[
\min F(\mathbf{Q}) = \sum_{i=1}^{N} \| Q_i \|, \quad \text{subject to } J(\phi) \leq J_0
\]  

(19)

where \( \| Q \| = \left\{ \int_0^T Q^2(t) dt \right\}^{1/2} \). Thus, \( F(\mathbf{Q}) \) is the total mass of the pollutant emitted within interval \((0,T)\) by \( N \) sources with emission rates \( Q_i(t) \). The solution of problem (19) is

\[
Q^*_i(t) = \gamma_i \alpha g(r_i,t) \|g(r_i,t)\|^2, \quad \gamma_i = m_i / (\sum_{i=1}^{N} m_i)
\]  

(20)

where \( \gamma_1 + \gamma_2 + ... + \gamma_N = 1 \), \( \gamma_i = m_i / (\sum_{i=1}^{N} m_i) \) is the part of the total mass of pollutant, emitted during time interval \((0,T)\) by the \( i \)-th source when all the sources are operating with emission rates \( Q_i(t) \) \((i=1,2,...,N)\), and

\[
\alpha = J_0 - \int_0^T g(r,0) \phi^0(r) dr > 0
\]  

(21)

5. General strategy for optimal emission control

Let \( \mathbf{Q}(t) = \{Q_1(t),...,Q_N(t)\} \) be nonstationary emission rates of \( N \) sources located at \( r_i \in D, i=1,2,...,N \). The functional

\[
F(\mathbf{Q}) = \frac{1}{2} \sum_{i=1}^{N} \gamma_i^2 \| Q_i - q_i \|^2 = \frac{1}{2} \sum_{i=1}^{N} \gamma_i^2 \int_0^T (Q_i - q_i)^2 dt
\]  

(22)

is defined on the set

\[
\Theta = \{ \mathbf{q}(t) : q_i(t) \geq 0, t \in [0,T], i=1,2,...,N; J(\phi) \leq J_0 \}
\]  

(23)

of such emission rates \( \mathbf{q}(t) \) that guarantee the compliance with the sanitary standard in a zone \( \Omega \):

\( J(\phi) \leq J_0 \). The aim of the optimal control is to find such emission rates \( \mathbf{Q}^*(t) \in \Theta \) that minimize the functional \( F(\mathbf{Q}) \) on the set \( \Theta \):

\[
F(\mathbf{Q}^*) = \inf_{\mathbf{Q} \in \Theta} F(\mathbf{Q})
\]  

(24)

The optimal solution \( \mathbf{Q}^*(t) \) is the smallest constraint on the intensity of source emissions. The weights \( \gamma_i \) in (22) are selected as follows. Denote by

\[
c_i = \int_0^T g(r_i,t)Q_i(t) dt > 0
\]  

the contribution of the \( i \)-th pollution source to the mean concentration \( J(\phi) \) in the monitoring zone \( \Omega \). Then \( f_i = c_i / (c_1 + ... + c_N) \) and \( \gamma_i = 1/ f_i \), \((i=1,2,...,N)\). Thus, a pollution source with less impact on the monitoring zone \( \Omega \) receives more weight, and therefore its optimal emission rate \( Q^*_i(t) \) will be closer to the original rate \( Q_i(t) \). Thus, control of emissions (22)-(24) is primarily aimed at reducing the intensity of emissions from sources that most pollute zone \( \Omega \).
Note that the solution to problem (24) critically depends on the parameter $\alpha$ (see (21)). Indeed, problem (23) has no solution if $\alpha < 0$, because the health standard cannot be met even if all production activity is stopped ($Q_i(t) \equiv 0$ for all $i$). The following three results were proved in [5].

**Theorem 1.** If $\alpha = 0$ then the optimal control problem (23) has only one solution:

$$Q_i'(t) = \begin{cases} 0, & \text{if } t \in I_i, \\ Q_i(t), & \text{if } t \in [0,T] \setminus I_i, \end{cases}$$

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

**Theorem 2.** If $\alpha > 0$ then the optimal control problem (23) has a unique solution $Q^* \in \Theta$ such that $Q_i'(t) \leq Q_i(t)$ ($0 \leq t \leq T$, $1 \leq i \leq N$) and $J(\phi) = J_0$.

If there is only one source in $D$, then Theorem 2 can be made more precise:

**Theorem 3.** Let there be only one source with emission rate $Q(t)$ located at the point $r_0 \in D$. If $J(\phi) > J_0$ and $\alpha > 0$ then

$$Q_i'(t) = Q_i(t) - \beta g(r_0,t) / \int_0^T g^2(r_0,t) dt,$$

is the only solution to the problem of optimal control (23) provided that it is a non-negative function in the interval $[0,T]$.

In connection with Theorem 2, the set of potential solutions (23) is reduced to

$$\Theta = \{ q_i(t) \geq 0, (i = 1, \ldots, N) \mid \sum_{i=1}^N g(r_i,t) q_i(t) dt = \alpha \}$$

This set is much smaller than (23) and therefore it is preferable in calculations. Typically, problem (25) is solved using the iterative optimization method with sequential estimation of the dynamic model $M$ [6], and therefore if the model $M$ is complex, this process is computationally intensive. However, the numerical solution of the optimal control problem can also be obtained using a highly efficient numerical algorithm of sequential orthogonal projections [5].

### 6. Example. Control of lead particle emissions

We now apply Theorem 3 for controlling lead particle emissions. The dispersion model (1)-(5) and adjoint model (9)-(11) are considered in the square domain $D = (0,2) \times (0,2)$ and four-hour interval $(0,T)$ where $T = 4$ h. Suppose that a single point source, located at point $r_0 = (1.8,0.2)$ emits lead particles. Note that all spatial dimensions in this example are shown in kilometers. For simplicity, we neglect the initial distribution of lead: $\phi^0(r) = 0$ in $D$. The coefficients of deposition and diffusion are $\sigma = 0.001$ h$^{-1}$ and $\mu = 0.04$ km$^2$ h$^{-1}$, respectively. The non-divergent wind velocity $U = (u,v)$ is defined by the stream function $\psi = xy$:

$$u = -\psi_y = -x, \quad v = \psi_x = y.$$ The mean lead concentration $J(\phi)$ is monitored in the zone $\Omega = [0,0.5] \times [0.5,1.0]$ during the whole interval $(0,T)$, that is, $\tau = 4$ h. The sanitary norm is $J_0 = 1.5 \mu$g m$^{-3}$ [7]. We will consider four different emission rates of the source:

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

$$Q_3(t) = \cos \pi t + 3.5, \quad Q_4(t) = \begin{cases} 3, & 0 \leq t < 1 \\ \frac{2}{3}(t-1) + 3, & 1 \leq t \leq 4 \end{cases}$$
For each $i$ ($i = 1, \ldots, 4$), the mean lead concentration $J_i(\phi)$ calculated in the zone $\Omega$ using the model (1)-(5) with emission rate $Q_i$ exceeds the sanitary standard $J_i$: $J_i(\phi)=2.11 \ \mu g/m^3$, $J_i(\phi)=2.02 \ \mu g/m^3$, $J_i(\phi)=1.97 \ \mu g/m^3$ and $J_i(\phi)=1.81 \ \mu g/m^3$. Therefore, in all four cases, the optimal control method (25) is applied. Figure 2 shows both the original emission rates $Q_i(t)$ and the optimal emission rates $q_{opt}(t)$ given by the control.

![Figure 2](image_url)

**Figure 2.** Temporal behavior of the original emission rates $Q_i(t)$ and optimal emission rates $q_{opt}(t)$ in four experiments.

As expected, for each $i$ ($i = 1, \ldots, 4$), $J_i(\phi)=J_i$ when optimal emission rate $q_{opt}(t)$ is used. Figure 2 shows that $q_{opt}(t) \leq Q_i(t)$ for all $t \in (0,4)$ and $1 \leq i \leq 4$. Besides, $q_{opt}(t) = Q_i(t)$ during the last hour interval (3 ≤ $t$ ≤ 4) when the value $g(\mathbf{r},t)$ of the adjoint model solution is equal to zero, and by virtue (15), the source emissions do not contribute to the pollution of zone $\Omega$. It is also interesting to note that in the interval 0 ≤ $t$ < 3, in which these values do not coincide, the temporal behavior of the optimal emission rate $q_{opt}(t)$ is similar to that of $Q_i(t)$ ($i = 1, \ldots, 4$). It means that the optimal strategy (25) does not require radical changes in the operation of the industrial source.

7. Identification of main parameters of unknown point sources

Dispersion models are commonly used to estimate the impact of pollutant emissions on air quality under various meteorological conditions. In addition, the previous sections have shown the importance of using the dispersion models and the adjoint approach in developing optimal emission control strategies. We will now show that the same methods can be used to evaluate the main parameters of unknown constant, instantaneous and nonstationary point pollution source.

Since problem (1)-(5) is linear, we can, without loss of generality, exclude from consideration all known sources in the domain $D$ and the pollutant concentration created by them. Therefore, we assume that only
one unknown source is active in $D$, and $\phi''(r) = 0$. Therefore, formula (16) for the concentration $\phi(R, t_j)$ of the pollutant at a monitoring site $R$ and moments $t_j$ is reduced to

$$\phi(R, t_j) = \int_0^{t_j} \phi(t) g_j(r^*_0, t) \, dt$$  \hspace{1cm} (26)$$

Also, assume that the measurements

$$\phi_j(R) = \phi(R, t_j) + \delta \phi_j, \quad j = 1, 2, \ldots, M,$$  \hspace{1cm} (27)$$

of the concentrations $\phi(R, t_j)$ contain errors $\delta \phi_j$ whose mean value is equal to zero:

$$\frac{1}{M} \sum_{j=1}^{M} \delta \phi_j = 0$$  \hspace{1cm} (28)$$

However, it should be noted the methods described below with minimal changes are also applicable in the general case when condition (28) is not satisfied.

A monitoring site $R$ is called *useful* if $\sum_{j=1}^{M} \phi_j(R) > 0$. In what follows, we will consider only useful monitoring sites.

**Case 1. An unknown constant point source.** The main parameters to be determined in this case are the constant intensity $Q_c$ and source location $r^*_0$. The pollutant concentration $\phi(R, t_j)$ at a monitoring site $R$ and moment $t_j$ is determined by formula (26), which in our case is reduced to

$$\phi(R, t_j) = Q \int_0^{t_j} g_j(r^*_0, t) \, dt$$  \hspace{1cm} (29)$$

where $g_j(r, t)$ is the solution of adjoint problem (9)-(11) in the interval $(0, t_j)$ obtained under the forcing $p(r, t) = \delta(r - R) \delta(t - t_j)$ and "initial" condition $g_j(r, t_j) = 0$ in $D$ because $g_j(r, t) = 0$ in $(t_j, T)$, $j = 1, 2, \ldots, M$. It follows from (29) and (27)-(28) that

$$\sum_{j=1}^{M} \phi(R, t_j) = Q \sum_{j=1}^{M} \int_0^{t_j} g_j(r^*_0, t) \, dt \quad \text{and} \quad \sum_{j=1}^{M} \phi_j(R) = \sum_{j=1}^{M} \phi(R, t_j)$$

Therefore, we have

$$Q_c = \left\{ \sum_{j=1}^{M} \phi_j(R) \right\} \left\{ \sum_{j=1}^{M} \int_0^{t_j} g_j(r^*_0, t) \, dt \right\}^{-1}$$  \hspace{1cm} (30)$$

Thus, if the location $r^*_0$ of the constant point source is known then (30) determines its emission rate $Q_c$. We will now show how to determine the source location $r^*_0$. Denote

$$\overline{\phi}_R = \sum_{j=1}^{M} \phi_j(R) \quad \text{and} \quad \overline{g}_R(r) = \int_0^T \left\{ \sum_{j=1}^{M} g_j(r, t) \right\} \, dt$$  \hspace{1cm} (31)$$

**Theorem 4.** Let $R_1, R_2, \ldots, R_N$ be useful monitoring sites. Then the source location $r^*_0$ is a zero of the function

$$\Phi(r) = \ln \left\{ 1 + \sum_{j=1}^{N} \left[ \overline{\phi}_{R_j}(r) - \overline{\phi}_{R_j}(r^*_0) \overline{g}_R(r) \right] \right\}$$  \hspace{1cm} (32)$$

Besides, due to (30) and (31), its emission rate is

$$Q_c = \overline{\phi}_R / \overline{g}_R(r^*_0).$$

**Proof.** By applying equation (30) to each monitoring site we obtain

$$Q_i = \overline{\phi}_{R_i} \left\{ \overline{g}_R(r^*_0) \right\}^{-1} \quad \text{and} \quad Q_c = \overline{\phi}_R \left\{ \overline{g}_R(r^*_0) \right\}^{-1}, \quad i = 1, \ldots, N$$

It means that
\[ \frac{\bar{\phi}_h}{\bar{g}_h(r'_0)} = \frac{\bar{\phi}_h}{\bar{g}_h(r'_0)}, \quad \text{or} \quad \left( \frac{\bar{\phi}_h}{\bar{g}_h(r'_0)} - \frac{\bar{\phi}_h}{\bar{g}_h(r'_0)} \right)^2 = 0, \quad i = 1, \ldots, N \]

Therefore, \( \sum_{i=1}^{N} \left[ \frac{\bar{\phi}_h}{\bar{g}_h(r'_0)} - \frac{\bar{\phi}_h}{\bar{g}_h(r'_0)} \right]^2 = 0 \) and \( \Phi(r'_0) = 0 \). Once the location \( r'_0 \) of the source is determined from equation \( \Phi(r'_0) = 0 \), the emission rate \( Q_c \) is calculated using Eq.(30). The theorem is proved.

**Case 2. An unknown instantaneous point source.** The main parameters to be determined in this case are the source location \( r'_* \), its intensity \( Q_c \) and the moment of emission \( t'_* \). In this case, \( Q(t) = Q_c \delta(t - t'_*) \), \( 0 < t'_* < T \). Summing again relations (29) over \( j \) from 1 to \( M \) and taking into account equations (27) and (28), we obtain

\[ Q = \left\{ \sum_{j=1}^{M} \phi_j(R) \right\} \left\{ \sum_{j=1}^{M} \int_{0}^{T} \delta(t - t'_*) g_j(r'_0, t) dt \right\}^{-1} \]

Since \( \int_{0}^{T} \delta(t - t'_*) g_j(r'_0, t) dt = g_j(r'_0, t'_*) \), we get

\[ Q = \left\{ \sum_{j=1}^{M} \phi_j(R) \right\} \left\{ \sum_{j=1}^{M} g_j(r'_0, t'_*) \right\}^{-1} \]

Denote

\[ \bar{g}_h(r, t) = \sum_{j=1}^{M} g_j(r, t) \]

**Theorem 5.** Let \( R, R_1, \ldots, R_N \) be useful monitoring sites. The point \( (r'_0, t'_*) \) is a zero of the function

\[ \Phi(r, t) = \ln \left\{ 1 + \sum_{i=1}^{N} \left[ \bar{\phi}_h \bar{g}_h(r, t) - \bar{\phi}_h \bar{g}_h(r, t) \right]^2 \right\} \]

Besides, due to (33) and (34), the emission intensity is \( Q_c = \frac{\bar{\phi}_h}{\bar{g}_h(r'_0, t'_*)} \).

**Proof.** By applying equation (33) for each useful monitoring site we obtain

\[ Q = \frac{\bar{\phi}_h}{\bar{g}_h(r'_0, t'_*)} \quad \text{and} \quad Q = \frac{\bar{\phi}_h}{\bar{g}_h(r'_0, t'_*)}, \quad i = 1, \ldots, N \]

i.e., \( \bar{\phi}_h \left\{ \bar{g}_h(r'_0, t'_*) \right\}^{-1} = \bar{\phi}_h \left\{ \bar{g}_h(r'_0, t'_*) \right\}^{-1} \) or \( \left[ \bar{\phi}_h \bar{g}_h(r'_0, t'_*) - \bar{\phi}_h \bar{g}_h(r'_0, t'_*) \right]^2 = 0, \quad i = 1, \ldots, N \). Therefore,

\[ \sum_{i=1}^{N} \left[ \bar{\phi}_h \bar{g}_h(r'_0, t'_*) - \bar{\phi}_h \bar{g}_h(r'_0, t'_*) \right]^2 = 0 \quad \text{and} \quad \Phi(r'_0, t'_*) = 0 \). Once the location \( r'_0 \) and emission moment \( t'_* \) is determined from equation \( \Phi(r'_0, t'_*) = 0 \), the intensity of emission \( Q_c \) is calculated from equation (33). The theorem is proved.

Note that the definition of the localization functions (32) and (35) in terms of logarithmic functions allows one to more accurately determine the zeros of these functions. Indeed, the feasible regions for the monitoring sites \( R_1, \ldots, R_N \) can be established as

\[ F_r = \{ r \in D : \prod_{i=1}^{N} g_i(r) > 0 \} \]

\[ F_t = \{ (r, t) \in D \times (0, T) : \prod_{i=1}^{N} g_i(r, t) > 0 \} \]

for a source of constant intensity and instantaneous source, respectively. The knowledge of the admissible spaces (36) is useful, since narrowing the search area for the zeros of localization functions reduces computational costs.
Case 3. An unknown nonstationary point source. This case, where both the intensity \( Q(t) \) and the location \( r_0 \) of a point source are unknown, is much more complicated than the previous two. Section 9 provides a variational method to determine the unknown emission rate \( Q(t) \) of a point source if its location \( r_0 \) is known. However, we now give a simple method for estimating the average intensity \( \bar{Q} \) of an unknown source during time interval \((0, T)\) if its location \( r_0^* \) in domain \( D \) is known. This value can give a rough estimate of the total mass of the pollutant emitted over the entire interval \((0, T)\). Indeed, summing formula (26) over moment \( t_j \) and using the mean value theorem we get

\[
\sum_{j=1}^{M} \phi_j(R) = \sum_{j=1}^{M} \phi(R, t_j) = \sum_{j=1}^{M} \int_{0}^{T} Q(t) g_j(r_0^*, t) \, dt
\]

\[
= \int_{0}^{T} Q(t) \left\{ \sum_{j=1}^{M} g_j(r_0^*, t) \right\} \, dt = \bar{Q} \sum_{j=1}^{M} \int_{0}^{T} g_j(r_0^*, t) \, dt
\]

where \( \bar{Q} \) can be considered as some average value of the emission intensity \( Q(t) \) in the interval \((0, T)\). Then

\[
\bar{Q} = \left( \sum_{j=1}^{M} \phi_j(R) \right) \left\{ \sum_{j=1}^{M} \int_{0}^{T} g_j(r_0^*, t) \, dt \right\}^{-1}
\]

(37)

8. Two examples of identification of parameters of unknown sources
Let us consider a one-dimensional dispersion model

\[
\frac{\partial \phi}{\partial t} - \mu \frac{\partial^2 \phi}{\partial x^2} + \sigma \phi = Q(t) \delta(x - x_0), \quad 0 < x < 1, \quad 0 < t < T
\]

\[
\mu \frac{\partial \phi}{\partial x}(0, t) = 0, \quad \mu \frac{\partial \phi}{\partial x}(1, t) = -\zeta \phi(1, t), \quad 0 < t < T
\]

\[
\phi(x, 0) = 0, \quad 0 < x < 1
\]

(38)

where \( \phi = \phi(x, t) \) is the concentration of a pollutant, \( \mu > 0, \sigma \geq 0 \) and \( Q(t) \) is the emission rate of a point source located at a point \( x_0 \) of the domain \( D = (0, 1) \). Conditions (38) mean that there is no pollution flux at \( x = 0 \) (the closed boundary), while at \( x = 1 \) the pollution flux is proportional to \( \phi \) with \( \zeta > 0 \) (the open boundary). As a result, the total mass of the pollutant in \( D \) increases due to non-zero emission rate \( Q(t) \) and decreases because of the pollution outflow at \( x = 1 \) and exponential decay of the pollutant concentration \( (\sigma > 0) \):

\[
\frac{\partial}{\partial t} \int_{0}^{1} \phi(x, t) \, dx = Q(t) - \zeta \phi(1, t) - \int_{0}^{1} \sigma \phi(x, t) \, dx
\]

The \( j \)-th adjoint model is

\[
-\frac{\partial g_{j}}{\partial t} - \mu \frac{\partial^2 g_{j}}{\partial x^2} + \sigma g_{j} = p(x, t), \quad 0 < x < 1, \quad 0 < t < T
\]

\[
\mu \frac{\partial g_{j}}{\partial x}(0, t) = 0, \quad \mu \frac{\partial g_{j}}{\partial x}(1, t) = -\zeta g_{j}(1, t), \quad 0 < t < T
\]

\[
g_{j}(x, T) = 0, \quad 0 < x < 1
\]

where \( p(x, t) = \delta(x - R) \delta(t - t_j) \) is the forcing, and \( R \) is the monitoring site in the domain \( D \). The following parameters were used: \( R = 0.2 \) km, \( \zeta = 1.0 \) km, \( \mu = 0.1 \) km\(^2\) h\(^{-1}\), \( \sigma = 0.01 \) h\(^{-1}\), \( T = 20 \) h, \( N = 1 \) and \( M = 200 \).
Example 1. Let us consider a constant source located at the point \( x_0 = 0.5 \text{ km} \) with intensity \( Q_s = 100 \text{ kg h}^{-1} \). Figures 3-5 show the localization function \( \Phi(x) \) for different monitoring sites \( R \) and \( R_i \). It should be noted that in all cases, the zero of \( \Phi(x) \) correctly determines the site of emission source. Besides, Theorem 4 allows us to correctly calculate the intensity \( Q_s = 100 \) of the source.

![Figure 3. Localization function \( \Phi(x) \). The monitoring sites are \( R = 0.2 \) and \( R_i = 0.4 \).](image)

Example 2. We now consider the case of an instantaneous source, which is located at the point \( x_0 = 0.7 \text{ km} \) and has intensity \( Q_s = 120 \text{ kg} \) at the moment \( t_s = 12 \text{ h} \). Figures 6-8 show the localization function \( \Phi(x,t) \) for different monitoring sites \( R \) and \( R_i \). It is seen that in all instances, the zeros of localization function correctly determine the site and the emission moment. Besides, Theorem 5 allows us to correctly calculate the intensity \( Q_s = 120 \) of the source.

![Figure 4. Localization function \( \Phi(x) \). The monitoring sites are \( R = 0.2 \) and \( R_i = 0.8 \).](image)
Figure 5. Localization function $\Phi(x)$. The monitoring sites are $R = 0.7$ and $R_i = 0.9$.

Figure 6. Cross-sections of the localization function $\Phi(x,t)$ for different moments $t_e$.

The monitoring sites are $R = 0.2$ and $R_i = 0.5$.

Figure 7. Cross-sections of the localization function $\Phi(x,t)$ for different moments $t_e$.

The monitoring sites are $R = 0.4$ and $R_i = 0.8$. 
9. Variational method for determining the intensity of nonstationary sources

Dispersion models are a fundamental tool for determining the main parameters of pollution sources using the measurements. Due to the presence of errors in the measurements, these inverse problems are usually ill-posed, since they may have several solutions or not have solutions. Moreover, solutions may be unstable with respect to variations in external and internal parameters of the problem. Therefore, to suppress instability and choose an appropriate solution to the inverse problem, special regularization methods should be used.

We now describe a variational method to determine the unknown nonstationary emission rate \( Q(t) \) of a point source if its location \( r_0 \) in domain \( D \) is known. Suppose that a time series \( \phi_j(R) = \phi(R, t_j) + \delta \phi_j, \quad j = 1, 2, \ldots, M \) of the pollutant concentrations is available at a monitoring site \( R \) (see (26)). Let us apply the Tikhonov regularization method [9] for the inverse problem:

\[
\begin{align*}
\text{minimize} & \quad J(q) = \frac{1}{2} \int_0^T [q(t)]^2 \, dt \\
\text{subject to:} & \quad -\varepsilon \leq \phi_j(R) - \int_0^T q(t) g_j(r_0, t) \, dt \leq \varepsilon, \quad j = 1, 2, \ldots, M
\end{align*}
\]

where \( q(t) \) is a nonnegative function in time interval \((0, T)\), besides, \( q(0) = q(T) = 0 \) (these zero conditions can always be met by expanding the interval \((0, T)\)). In each condition (40), the measurement error is limited by a value \( \varepsilon \), which expands the feasibility space and affects the smoothness of the numerical solution \( Q_j(t) \). Experiments show that optimal value of \( \varepsilon \) is \( \varepsilon^* = \max_j ||\delta \phi_j|| \).

A discrete problem approximating the variational formulation (39)-(40) with the second order of accuracy can be written as a quadratic programming problem:

\[
\begin{align*}
\text{minimize} & \quad J(q) = 0.5 (\Delta t)^{-1} \, q^T B q \\
\text{subject to:} & \quad -\varepsilon \leq \phi_j(R) - \sum_{l=1}^M a_{jl} q_l \leq \varepsilon, \quad j = 1, 2, \ldots, M \\
& \quad q_l \geq 0, \quad l = 1, \ldots, M - 1, \quad q_0 = q_M = 0
\end{align*}
\]
where $B$ is a tridiagonal, symmetric and positive definite matrix with $B_{ii} = 2$ and $B_{i,i+1} = B_{i+1,i} = -1$; the mesh nodes $t_j = j \Delta t$ in the interval $[0,T]$ are the measurement moments, $l = 0,1,\ldots,M$; vector $q = (q_1,\ldots,q_{M+1})^T$ where $q_i = q(t_i)$ is the solution, and

$$a_{jj} = 0.5 \Delta t \, g_j(r_c,t_j), \quad j = 1,\ldots,M-1$$

$$a_{jj} = \Delta t \, g_j(r_c,t_j), \quad 1 < j < M, \quad 1 \leq l < j$$

Problem (41)-(42) has a solution because its feasibility set (42) is nonempty and compact in the vector space $\mathbb{R}^{M+1}$, and function $J(q)$ is continuous. Since $J(q)$ is strictly convex, the solution of problem (41)-(42) is unique [1] and can be found with the quadprog routine of MATLAB.

**Example. Identification of nonstationary emission rate** $Q(t)$. We consider a 1D version of problems (1)-(5) and (9)-(11) in domain $D = (0,1)$ and interval $(0,T)$, where $T = 40$, using the following dimensionless parameters: $U = 0.85, \mu = 0.5, \sigma = 0.1, \zeta = 1.0, r_c = 0.3$ and $R = 0.8$. Also, $Q(t) = 100 r e^{-0.5 t} \sin^2 t$ if $0 \leq t \leq 4\pi$, and $Q(t) = 0$ otherwise. The graph of the emission rate $Q(t)$ and the solution $\phi(R,t)$ of problem (1)-(5) at the monitoring site $x = R$ are shown in Figure 9. Since the conditions of atmospheric dispersion are stationary, the operators of the direct and adjoint problems do not depend on time, and therefore $g_j(r_c,t) = g_j(r_c,t_j) \delta(t - t_j)$ in $(0,t_j)$ for every $j$ ($j = 1,2,\ldots,M$) where $g_j(r_c,t)$ known as the basic kernel is the adjoint solution of 1D problem (9)-(11) under the forcing $p(r,t) = \delta(r - R) \delta(t - T)$. Thus, each adjoint function $g_j(r_c,t)$ is a displacement in time of the basic kernel. The basic kernel $g_j(r_c,t)$ and two adjoint functions $g_j(r_c,t)$ are shown in Figure 10.

![Figure 9. Emission rate $Q(t)$ and concentration $\phi(R,t)$.](image-url)
Once the adjoint functions have been obtained, we can solve the quadratic programming problem (41)-(42). Errors $\delta \phi_j$ in the synthetic time series $\{\phi_j(R)\}_{j=0}^m$ (see (27)) are randomly chosen values from a uniform distribution in the interval $(-0.5, 0.5)$. The amplitudes of errors were normalized so as not to exceed 15% of the maximum value of the function $\phi(R, t)$. Figure 11 shows the behavior of the recoverable function $Q(t)$ and three regularized solutions $Q_*(t)$ as $\varepsilon \rightarrow \varepsilon^*$ approaches $\varepsilon^*$ from the right, where $\varepsilon^* = \max_j |\phi_j|$, and $\varepsilon = 2.0, 1.6, 1.002$. The numerical experiments also show that solution of (41)-(42) becomes smoother and tends to zero if $\varepsilon \rightarrow +\infty$ (since the feasibility set (42) expands to such an extent that it contains the global minimum of objective function). Besides, for $\varepsilon = \varepsilon^*$ we get the best approximation of $Q(t)$ which the method gives.

Figure 10. Basic kernel $g_a(t_x, t)$ and adjoint functions $g_j(t_x, t)$ for $t_j = 30$ and $t_j = 35$.

Figure 11. Approximation of recoverable function $Q(t)$ by regularized solutions $Q_*(t)$ as $\varepsilon \rightarrow \varepsilon^*$. 
10. Conclusions
In this work, the dispersion of a pollutant from industrial point sources in a limited area is described by the advection-diffusion equation. Direct and adjoint estimates of the concentration of the pollutant at the monitoring sites are obtained. Optimal control strategies based on using the adjoint estimates are developed to prevent violations of existing sanitary regulations by timely reduction of emissions from the sources. We used here two advantages of the adjoint approach: 1) the adjoint estimates depend explicitly on both the number, location and intensity of sources, and the initial concentration of the pollutant in the area; 2) solutions of adjoint problems serve in such assessments as the weighting functions providing valuable information about the contribution of each source to the concentration of the pollutant at the monitoring site. These properties make the adjoint estimates efficient for studying the sensitivity of the problem to variations in the emission rates and initial conditions, and for developing emission control strategies. Also, methods are developed for the identification of the main parameters of an unknown point source in the cases when its intensity is constant, instantaneous or nonstationary. The effectiveness of the methods is illustrated by simple examples.

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