

Control and Identification of Air Pollution Sources

YURI N. SKIBA*, DAVID PARRA-GUEVARA
Institute of Atmospheric Sciences and Climate Change
National Autonomous University of Mexico
Av. Universidad 3000, CU/UNAM, C.P. 04510 Mexico City
MEXICO

*Corresponding Author

Abstract: A pollutant model and its adjoint model for a bounded zone with an open boundary are considered; dual estimates of pollutant concentrations are derived, and a method for the real-time control of emissions is presented. Methods are proposed for identifying the intensity and location of a new, unknown pollution source.

Key-Words: Air pollution model, direct and adjoint pollutant assessment, control of emission rates, determination of strength and position of a new source

Received: April 17, 2026. Revised: June 23, 2026. Accepted: July 26, 2026. Published: October 22, 2026.

1 Two-dimensional dispersion problem

Let us assume that D is a two-dimensional bounded area with an open border S . Let us assume that pollution sources are located at points $\mathbf{r}_i = (x_i, y_i)$ of area D ($i=1, 2, \dots, N$). Let $\psi(\mathbf{r}, t)$ denote the pollutant concentration at $\mathbf{r} = (x, y)$ and at time t . For simplicity, the dispersion of the pollutant in $D \times (0, T)$ is studied using a 2D advection-diffusion equation

$$\frac{\partial \psi}{\partial t} + \mathbf{U} \cdot \nabla \psi + \sigma \psi - \nabla \cdot \mu \nabla \psi = f \quad (1.1)$$

where

$$f = \sum_{i=1}^N Q_i(t) \delta(\mathbf{r} - \mathbf{r}_i), \quad (1.2)$$

$Q_i(t)$ and $\mathbf{r}_i$ are the pollution output and location of the i th source; $\mathbf{U} \equiv \mathbf{U}(\mathbf{r}, t)$ is the known nondivergent wind velocity (climatic or calculated using a model), that is,

$$\nabla \cdot \mathbf{U} = 0, \quad (1.3)$$

$\sigma(\mathbf{r}, t) > 0$ determines the decay rate of the concentration contaminant ψ as a result of various physical and chemical processes, and $\mu(\mathbf{r}, t) > 0$. The initial condition for equation (1.1) is

$$\psi(\mathbf{r}, 0) = \psi^0(\mathbf{r}) \quad (1.4)$$

As a rule, the flux of the pollutant across S is unfamiliar. To formulate a well-defined problem according to Hadamard [3], care must be taken when using boundary conditions [4, 5]. We now formulate boundary conditions that are acceptable from both physical and mathematical points of view. Let

$U_n = \mathbf{U} \cdot \mathbf{n}$ be the projection of the velocity $\mathbf{U}$ onto the unit outward normal $\mathbf{n}$ to the boundary. We divide the boundary S into two parts: the part S^+ (where $U_n \geq 0$, and the pollution flux is directed out of the region D) and the part S^- (where $U_n < 0$, and the pollution flux is directed into D) (Figure 1). And on these boundaries, we will impose the following conditions:

$$\mu \frac{\partial \psi}{\partial n} - U_n \psi = 0 \quad \text{on } S^- \quad (1.5)$$

$$\mu \frac{\partial \psi}{\partial n} = 0 \quad \text{on } S^+ \quad (1.6)$$

According to condition (1.5), the total flux of the pollutant (both diffusive and advective) across S^- is zero. On the other hand, condition (1.6) means that the diffusion flux $\mu \partial \psi / \partial n$ across S^+ is negligible compared to the advective flux $U_n \psi$. In the limiting case when $\mu = 0$ (there is no diffusion), condition (1.5) reduces to the condition $\psi = 0$ (there is no contamination on S^-), and condition (1.6) vanishes, as expected. Indeed, the problem of pure advection ($\mu = \sigma = 0$) does not require a condition on the outflow part S^+ where the solution ψ is determined by the method of characteristic lines [2]. We will see later that problem (1.1)-(1.6) is also well posed from a mathematical point of view, since it has a unique solution that depends continuously on $\psi^0(\mathbf{r})$, and the number N , the strength $Q_i(t)$ and the location $\mathbf{r}_i$ of sources.

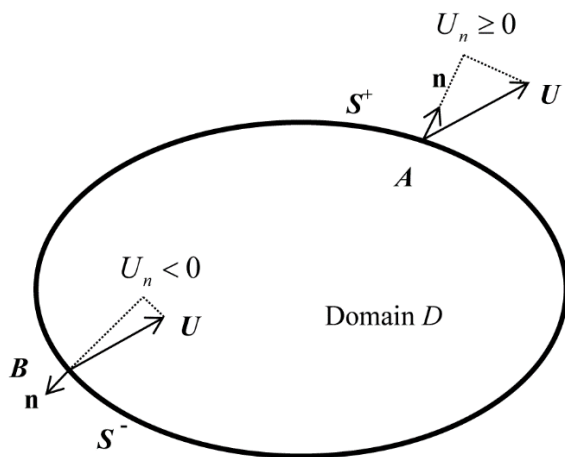


Fig. 1. A limited industrial region D with border $S = S^+ \cup S^-$.

2 Integral balance equations

Integrating equation (1.1) over D and considering (1.3), (1.5) and (1.6), we obtain an equation for the total mass of the pollutant

$$\frac{d}{dt} \int_D \psi \, d\mathbf{r} = \sum_{i=1}^N Q_i - \int_D \sigma \psi \, d\mathbf{r} - \int_{S^+} U_n \psi \, dS \quad (2.1)$$

Now, let us multiply equation (1.1) by ψ and integrate the resulting equation over D using (1.3), (1.5) and (1.6). Then we obtain

$$\begin{aligned} \frac{d}{dt} \int_D \psi^2 \, d\mathbf{r} &= 2 \sum_{i=1}^N Q_i(t) \psi(\mathbf{r}_i, t) \\ &- 2 \int_D (\sigma \psi^2 + \mu |\nabla \psi|^2) \, d\mathbf{r} - \int_{S^+} U_n \psi^2 \, dS + \int_{S^-} U_n \psi^2 \, dS \end{aligned} \quad (2.2)$$

Equation (2.2) describes the behavior of the solution norm $\|\psi\| = \left(\int_D \psi^2 \, d\mathbf{r} \right)^{1/2}$. Given that $U_n < 0$ on S^- and $U_n \geq 0$ on S^+ , equation (2.2) accepts the form

$$\begin{aligned} \frac{d}{dt} \int_D \psi^2 \, d\mathbf{r} &= 2 \sum_{i=1}^N Q_i \psi(\mathbf{r}_i, t) \\ &- 2 \int_D (\sigma \psi^2 + \mu |\nabla \psi|^2) \, d\mathbf{r} - \int_S |U_n| \psi^2 \, dS \end{aligned} \quad (2.3)$$

Thus, the total pollutant concentration, as well as the solution norm, increase due to the action of pollution sources ($Q_i(t) > 0$) and decrease as a result of dissipation ($\sigma > 0$), diffusion ($\mu > 0$), and the transport of the pollutant across the region boundary D .

If $Q_i(t) = 0$ for all i (there are no active pollution sources in D), both $\int_D \psi \, d\mathbf{r}$ and $\|\psi\|$ decrease with

time. Moreover, if dissipation is also absent ($\sigma = 0$, $\mu = 0$) and $U_n = 0$ on S (this is, of course, an idealized case), then

$$\frac{d}{dt} \int_D \psi \, d\mathbf{r} = 0, \quad \frac{d}{dt} \int_D \psi^2 \, d\mathbf{r} = 0 \quad (2.4)$$

In other words, we have at our disposal two conservation laws for verifying numerical algorithms and computer programs [10].

3 Positive definiteness of the operator

Let us demonstrate that the operator

$$A\psi = \mathbf{U} \cdot \nabla \psi + \sigma \psi - \nabla \cdot (\mu \nabla \psi) \quad (3.1)$$

associated with problem (1.1)-(1.6) is positive definite. Its domain is the set

$$\Phi = \{ \psi \in C^2(\bar{D}) \mid \mu \frac{\partial \psi}{\partial \mathbf{n}} - U_n \psi = 0 \text{ on } S^- \text{ and} \}$$

$$\mu \frac{\partial \psi}{\partial \mathbf{n}} = 0 \text{ on } S^+ \} \subset L_2(\bar{D}) \quad (3.2)$$

where $\bar{D} = D \cup S$. Let $L_2(\bar{D})$ be the Hilbert space with the inner product

$$(\psi, g) = \int_D \psi(\mathbf{r}) g(\mathbf{r}) \, d\mathbf{r}$$

and the norm $\|\psi\| = \left(\int_D \psi^2 \, d\mathbf{r} \right)^{1/2}$. Then

$$\begin{aligned} (A\psi, \psi) &= \int_D \psi \mathbf{U} \cdot \nabla \psi \, d\mathbf{r} \\ &+ \int_D \sigma \psi^2 \, d\mathbf{r} - \int_D \psi \nabla \cdot (\mu \nabla \psi) \, d\mathbf{r} \end{aligned} \quad (3.3)$$

Since $\nabla \cdot \mathbf{U} = 0$, we can write

$$\nabla \cdot (\psi^2 \mathbf{U}) = 2\psi \mathbf{U} \cdot \nabla \psi.$$

Also,

$$\nabla \cdot (\psi \mu \nabla \psi) = \psi \nabla \cdot (\mu \nabla \psi) + \mu |\nabla \psi|^2$$

Therefore, using the divergence theorem, we obtain

$$\begin{aligned} \int_D \psi \mathbf{U} \cdot \nabla \psi \, d\mathbf{r} &= \frac{1}{2} \int_S \psi^2 \mathbf{U} \cdot \mathbf{n} \, dS \\ &= \frac{1}{2} \left[\int_{S^+} \psi^2 U_n \, dS + \int_{S^-} \psi^2 U_n \, dS \right] \end{aligned} \quad (3.4)$$

and

$$\begin{aligned} - \int_D \psi \nabla \cdot (\mu \nabla \psi) \, d\mathbf{r} &= \int_D \mu |\nabla \psi|^2 \, d\mathbf{r} \\ &- \int_S \psi \mu \nabla \psi \cdot \mathbf{n} \, dS \end{aligned} \quad (3.5)$$

Let us use now that $S = S^+ \cup S^-$. Then (1.5) and (1.6) lead to

$$\begin{aligned} - \int_D \psi \nabla \cdot (\mu \nabla \psi) \, d\mathbf{r} &= \int_D \mu |\nabla \psi|^2 \, d\mathbf{r} \\ &- \int_{S^-} \psi^2 U_n \, dS \end{aligned} \quad (3.6)$$

Using formulas (3.4) and (3.6) in (3.3) leads to

$$(A\psi, \psi) = \int_D \{\sigma \psi^2 + \mu |\nabla \psi|^2\} d\mathbf{r} + \frac{1}{2} \int_S \psi^2 |U_n| dS > 0 \quad (3.7)$$

So, A is positive definite operator. Note that A is positive semidefinite if $\sigma = 0$ and $U_n = 0$ at S , and antisymmetric if $\sigma = 0$, $\mu = 0$ and $U_n = 0$ at S .

4 Uniqueness and stability of the solution

Let us write the problem (1.1)-(1.6) in operator form:

$$\frac{\partial \psi}{\partial t} + A\psi = f \quad (4.1)$$

$$\psi(0) = \psi^0 \quad (4.2)$$

where $A : \Phi \subset H \rightarrow H$ is a positive semidefinite operator: $(A\psi, \psi) \geq 0$ for any $\psi \neq 0$. Then

$$\left(\frac{\partial \psi}{\partial t}, \psi\right) = (f, \psi) - (A\psi, \psi) \quad (4.3)$$

And

$$\left(\frac{\partial \psi}{\partial t}, \psi\right) \leq \|f\| \|\psi\| \quad (4.4)$$

where $\|\psi\| = \sqrt{(\psi, \psi)}$. The inequality (4.4) leads to

$$\frac{d}{dt} \|\psi\| \leq \|f\| \quad (4.5)$$

Integrating (4.5) over time interval $(0, t)$, we obtain

$$\|\psi\| \leq \int_0^t \|f\| d\tau + \|\psi^0\| \quad (4.6)$$

We used condition (4.2) in (4.6). Then

$$\|\psi\| \leq T \cdot \max_{0 \leq t \leq T} \|f(\mathbf{r}, t)\| + \|\psi^0\| \quad (4.7)$$

Due to the linearity of the problem, the solution is stable against perturbations.

Similar arguments guarantee the uniqueness of the solution. Indeed, if there are two solutions ψ_1 and ψ_2 to problem (4.1)-(4.2) then $\delta\psi = \psi_1 - \psi_2$ is also a solution with $\delta\psi^0 = 0$ and $\delta f = 0$. Therefore, due to (4.7), $\delta\psi \equiv 0$, i.e., both solutions coincide.

Thus, $(A\psi, \psi) \geq 0$ implies the stability. It should be noted that $(A\psi, \psi) \geq 0$ is also a necessary condition for stability. Indeed, a perturbation in the form of an eigenfunction corresponding to the negative eigenvalue will grow over time.

Note that a similar result holds for the discrete problem obtained after discretizing problem (4.1) –

(4.2). Furthermore, this property enables the use of the splitting method to construct implicit and unconditionally stable schemes designed for the efficient solution of 2D and 3D dispersion problems [10].

5 Adjoint problem associated with the dispersion problem

Now let us formulate, in the same domain $D \times (0, T)$, another problem related to the problem (1.1)-(1.6) [4, 5]:

$$-\frac{\partial g}{\partial t} - \mathbf{U} \cdot \nabla g + \sigma g - \nabla \cdot (\mu \nabla g) = p(\mathbf{r}, t) \quad (5.1)$$

$$g(\mathbf{r}, T) = 0 \quad \text{in } D \quad (5.2)$$

$$\mu \frac{\partial g}{\partial n} = 0 \quad \text{on } S^- \quad (5.3)$$

$$\mu \frac{\partial g}{\partial n} + U_n g = 0 \quad \text{on } S^+ \quad (5.4)$$

with the same velocity $\mathbf{U}$ as in equation (1.1) and $p(\mathbf{r}, t)$ is a forcing, which we will define later.

Let us compare problems (1.1)-(1.6) and (5.1)-(5.4) in the case when $f(\mathbf{r}, t) \equiv 0$ and $p(\mathbf{r}, t) \equiv 0$. It is evident that after substitutions $t' = T - t$ and $\mathbf{U}' = -\mathbf{U}$, problem (5.1)-(5.4) takes the same form as the dispersion problem (1.1)-(1.6). As a result, the output boundary S^+ (or input boundary S^-) of problem (1.1)-(1.6) becomes the input boundary S^- (output boundary S^+) of problem (5.1)-(5.4). That is precisely why boundary conditions (1.5) and (1.6) are replaced by boundary condition (5.3) and (5.4). Moreover, it follows from this that the problem (5.1) - (5.4) is well-posed in the sense of Hadamard only if it is solved in the reverse time direction: from $t = T$ to $t = 0$.

Thus, the uniqueness and stability of a solution to the problem (5.1) - (5.4) directly follows from the results obtained in section 4. It can be shown that the operator of problem (5.1) - (5.4) is adjoint to the operator of problem (1.1)-(1.6). Therefore, in what follows we will call (5.1) - (5.4) the adjoint problem.

6 Dual estimates of pollutant concentrations

In the following, we will refer to estimates of the pollutant concentration based on the solution to the dispersion problem (1.1)-(1.6) as direct estimates. However, in this section, we derive alternative and equivalent adjoint counterparts, using the solutions to the adjoint problems (5.1)-(5.4).

To this end, we multiply equations (5.1) and (1.1) respectively by $\psi(\mathbf{r}, t)$ and $g(\mathbf{r}, t)$, subtract one equation from the other, and then integrate the result over $D \times (0, T)$. Accounting the conditions (1.5)-(1.6) and (5.3)-(5.4), the forcing (1.2), and the initial condition (5.2), we obtain

$$\int_0^T \int_D p(\mathbf{r}, t) \psi(\mathbf{r}, t) d\mathbf{r} dt = \sum_{i=1}^N \int_0^T g(\mathbf{r}_i, t) Q_i(t) dt + \int_D g(\mathbf{r}, 0) \psi^0(\mathbf{r}) d\mathbf{r} \quad (6.1)$$

Let us consider two special forms of the forcing $p(\mathbf{r}, t)$:

1) If we set $p(\mathbf{r}, t) = \delta(t - t_j) \delta(\mathbf{r} - \mathbf{r}_j)$ in (5.1) then (6.1) yields another (equivalent) estimate of the pollutant concentration at the monitoring point $(\mathbf{r}_j, t_j)$:

$$\psi(\mathbf{r}_j, t_j) = \sum_{i=1}^N \int_0^T g(\mathbf{r}_i, t) Q_i(t) dt + \int_D g(\mathbf{r}, 0) \psi^0(\mathbf{r}) d\mathbf{r} \quad (6.2)$$

2) let $\tau \in [0, T]$ and $\Omega \subseteq D$ be a monitoring zone with area $|\Omega|$. If

$$p(\mathbf{r}, t) = \begin{cases} 1/(\tau|\Omega|), & \text{if } (\mathbf{r}, t) \in (T - \tau, T) \times \Omega \\ 0, & \text{otherwise} \end{cases} \quad (6.3)$$

in equation (5.1) then relation (6.1) yields another (equivalent) estimate of the mean pollutant concentration in the domain $\Omega \times (T - \tau, T)$:

$$\frac{1}{\tau|\Omega|} \int_{T-\tau}^T \int_{\Omega} \psi(\mathbf{r}, t) d\mathbf{r} dt = \sum_{i=1}^N \int_0^T g(\mathbf{r}_i, t) Q_i(t) dt + \int_D g(\mathbf{r}, 0) \psi^0(\mathbf{r}) d\mathbf{r} \quad (6.4)$$

Thus, we have two direct estimates

$$J(\psi) = \psi(\mathbf{r}_j, t_j) \text{ and}$$

$$J(\psi) \equiv \frac{1}{\tau|\Omega|} \int_{T-\tau}^T \int_{\Omega} \psi(\mathbf{r}, t) d\mathbf{r} dt \quad (6.5)$$

and two adjoint estimates

$$J(\psi) = \sum_{i=1}^N \int_0^T g(\mathbf{r}_i, t) Q_i(t) dt + \int_D g(\mathbf{r}, 0) \psi^0(\mathbf{r}) d\mathbf{r} \quad (6.6)$$

appearing on the right side of (6.2) and (6.4) which use the solutions of two different problems (5.1)-(5.4).

The adjoint estimate (6.6) is important because it provides an explicit dependence of the pollutant concentration $J(\psi)$ on the source emission intensities $Q_i(t)$ over interval $(0, T)$ and on the

initial pollutant distribution $\psi^0(\mathbf{r})$ in D . Moreover, the adjoint solution $g(\mathbf{r}, t)$ is nonnegative and independent of $Q_i(t)$ and $\psi^0(\mathbf{r})$. Consequently, the values $g(\mathbf{r}_i, t)$ and $g(\mathbf{r}, 0)$ serve in estimate (6.6) as weight functions (or influence functions) characterizing the contribution of each pollution source and the initial pollutant distribution $\psi^0(\mathbf{r})$.

It should be noted that as the length of the interval $(0, T - \tau)$ increases, the influence of the initial pollutant concentration $\psi^0(\mathbf{r})$ decreases. Indeed, due to (6.3), $p(\mathbf{r}, t) \equiv 0$ if $t \in (0, T - \tau)$, and due to dissipation ($\sigma > 0$), the quantity $g(\mathbf{r}, 0)$ in (6.6) tends to zero as $(T - \tau) \rightarrow \infty$.

We also note that direct estimates use the solution of dispersion problem (1.1)-(1.6), which makes it possible to analyze the environmental situation in any part of the region $D \times (0, T)$. On the other hand, solutions to adjoint problems (5.1)-(5.4), calculated for a point $(\mathbf{r}_j, t_j) \in D \times (0, T)$ or environmentally significant zone Ω , do not depend on the number of pollution sources N , as well as on their intensity $Q_i(t)$ and location $\mathbf{r}_i$. This feature makes adjoint estimates very effective for studying the N -dependence, $Q_i(t)$ -dependence and/or $\mathbf{r}_i$ -dependence of concentration $J(\psi)$ in the zone Ω [6, 7]. In particular, they are necessary when solving the problem of optimal control of industrial emissions or identifying the intensity and location of unknown pollution sources. In general, dual estimates complement each other quite well when solving various pollution problems.

7 Emission control

Typically, short-term control is conducted over a brief period - ranging from a few hours to a few days - and is applied to relatively small areas. Such control is usually associated with periods of atmospheric stability (calm conditions, atmospheric inversions). Measures taken during such control usually include actions leading to an immediate reduction in pollutant emissions. Besides, the particular goal of monitoring under conditions of atmospheric stability is to maintain pollutant concentrations within sanitary limits.

Let us formulate the mathematical problem of such management. Assume that a dispersion model $\mathbf{A}^A: \bar{Q} \rightarrow \psi_{\bar{Q}}$ is used for the forecasting of pollutant concentrations ψ in $D \times [0, T]$,

where $\vec{Q} = \{Q_1, Q_2, \dots, Q_N\}$ is composed of time-varying discharge levels Q_i from N sources positioned at $\mathbf{r}_i \in D$. Let $|\Omega|$ be an area of environmentally sensitive region $\Omega \subset D$. Let us assume that the result obtained using the predictive model $\mathcal{M}$ with emission rates $\vec{Q}$ is unsatisfactory, i.e., $J(\psi_{\vec{Q}}) > J_0$ where $J(\psi_{\vec{Q}})$ is the mean pollutant concentration in $\Omega \times [T - \tau, T]$, and J_0 is the sanitary limit. This result implies that the discharge levels $\vec{Q} = \{Q_1, Q_2, \dots, Q_N\}$ are excessive, and the regulatory task is to determine reduced discharge levels $\vec{Q}^* = \{Q_1^*, Q_2^*, \dots, Q_N^*\}$ such that a re-forecast with new levels $\vec{q}$ for the same time period $[0, T]$ yields the desired result:

$$J(\psi_{\vec{Q}^*}) \leq J_0 \quad (7.1)$$

For simplicity, we will use $J(\psi)$ in place of $J(\psi_{\vec{Q}})$. To meet the condition $J(\psi) \leq J_0$ the emission intensity $\vec{Q}$ must satisfy

$$\sum_{i=1}^N \int_0^T g(\mathbf{r}_i, t) Q_i(t) dt \leq \alpha \quad (7.2)$$

where

$$\alpha = J_0 - \int_D g(\mathbf{r}, 0) \psi^0(\mathbf{r}) d\mathbf{r} \quad (7.3)$$

is the parameter characterizing the possibility of controlling emissions [6]. Indeed, if $\alpha = 0$ then the condition (7.2) can be satisfied only if $\vec{Q} \equiv 0$ in $(0, T)$. This means a complete cessation of production activity. If $\alpha < 0$, then the control problem has no solution.

The case $\alpha > 0$ is of interest. It occurs when the pollutant concentration ψ^0 accumulated over a preceding period is relatively low.

8 General problem of optimal control

Let $\vec{q}(t) = \{q_1(t), q_2(t), \dots, q_N(t)\}$ be an element of a space $\mathbf{H}$ with the norm

$$\|\vec{q}\| = \left(\sum_{i=1}^N \|q_i\|_{L_2[0, T]}^2 \right)^{1/2} = \left(\sum_{i=1}^N \int_0^T q_i^2(t) dt \right)^{1/2}.$$

Define the functional

$$F(\vec{q}) = \|\vec{Q} - \vec{q}\|^2 = \sum_{i=1}^N \int_0^T (Q_i - q_i)^2 dt \quad (8.1)$$

on the set

$$\Theta = \left\{ q_i(t) \in L_2[0, T] \mid q_i \geq 0, (i=1, \dots, N) \text{ and } J(\psi_{\vec{q}}) \leq J_0 \right\} \quad (8.2)$$

where the components $q_i(t)$ of $\vec{q}(t)$ are new emission levels that ensure adherence to sanitary norm in the zone Ω : $J(\psi_{\vec{q}}) \leq J_0$.

The optimal control problem consists in determining such $\vec{Q}^* \in \Theta$ that

$$F(\vec{Q}^*) = \inf_{\vec{q} \in \Theta} F(\vec{q}) \quad (8.3)$$

It should be noted that the components $Q_i^*(t)$ impose minimal constraints on production activities. Typically, the variational problem (8.3) is solved using successive approximations based on the model $\mathcal{M}$. Overall, this process is not highly efficient, as it necessitates a large volume of computations. Therefore, we now employ an adjoint approach without re-evaluating the model $\mathcal{M}$.

Theorem 1. Let $\alpha > 0$. Then the optimal control problem (8.3) has a unique solution.

Proof. First of all, define the admissible set Θ as follows:

$$\Theta = \left\{ q_i(t) \in L_2[0, T] \mid q_i \geq 0, (i=1, \dots, N) \text{ and } \sum_{i=1}^N \int_0^T g(\mathbf{r}_i, t) q_i(t) dt \leq \alpha \right\} \quad (8.4)$$

The set Θ is convex. Indeed, let $\vec{q}_1, \vec{q}_2 \in \Theta$ and $0 \leq \lambda \leq 1$. Then

$$\sum_{i=1}^N \int_0^T g(\mathbf{r}_i, t) \{ \lambda q_{1i}(t) + (1 - \lambda) q_{2i}(t) \} dt \leq \alpha$$

In addition,

$$F(\vec{q}) = \sum_{i=1}^N \|Q_i - q_i\|_{L_2[0, T]}^2$$

is strictly convex in Θ . These results guarantee the uniqueness of the solution. Q.E.D.

We now prove the existence of a solution.

Lemma 1. The admissible set Θ is closed in $\mathbf{H}$.

Proof. We demonstrate that $\Theta = \bar{\Theta}$. Let $\vec{q}_0 \in \bar{\Theta}$.

Then there is a sequence $\{\vec{q}_k\} \subset \Theta$ with the property that

$$\|\vec{q}_k - \vec{q}_0\| \rightarrow 0 \text{ as } k \rightarrow \infty.$$

We demonstrate by reductio ad absurdum that

$$q_{0i} \geq 0 \quad \forall i \ (i = 1, \dots, N).$$

Suppose that for some j , $q_{0j} < 0$ in a set $I \subset [0, T]$ of positive measure: $|I| > 0$. Then

$$\begin{aligned} \|\vec{q}_k - \vec{q}_0\|^2 &= \sum_{i=1}^N \int_0^T [q_{ki}(t) - q_{0i}(t)]^2 dt \\ &\geq \int_I [q_{kj}(t) - q_{0j}(t)]^2 dt \\ &\geq \int_I q_{0j}^2(t) dt = l > 0 \end{aligned}$$

for every k which contradicts the convergence of the sequence $\{\vec{q}_k\}$. Hence, $\|g(\mathbf{r}_i, t)\|_{L_2[0, T]}$ is finite, and

$$\|q_{ki}(t) - q_{0i}(t)\|_{L_2[0, T]} \rightarrow 0 \text{ as } k \rightarrow \infty.$$

By the Schwarz inequality,

$$\sum_{i=1}^N \int_0^T g(\mathbf{r}_i, t) q_{ki}(t) dt \rightarrow \sum_{i=1}^N \int_0^T g(\mathbf{r}_i, t) q_{0i}(t) dt$$

and taking the limit in

$$\sum_{i=1}^N \int_0^T g(\mathbf{r}_i, t) q_{ki}(t) dt \leq \alpha \text{ as } k \rightarrow \infty$$

leads to

$$\sum_{i=1}^N \int_0^T g(\mathbf{r}_i, t) q_{0i}(t) dt \leq \alpha, \text{ i.e.,}$$

$$\vec{q}_0 \in \Theta. \text{ Q.E.D.}$$

Lemma 2 [1]. *In a uniformly convex Banach space, a closed convex set contains exactly one point closest to a given point.*

Theorem 2. *The optimal control problem (8.3) has a solution.*

Proof. The Hilbert space $\mathbf{H}$ is a uniformly convex Banach space [1]. Furthermore, the set $\Theta \subset \mathbf{H}$ is closed and convex according to Theorem 1 and Lemma 1, and $\vec{Q} \notin \Theta$ since

$$\sum_{i=1}^N \int_0^T g(\mathbf{r}_i, t) Q_i(t) dt > \alpha \quad (8.5)$$

Then, according to Lemma 2, there exists a point $\vec{Q}^* \in \Theta$ minimizing the distance between Θ and $\vec{Q}$. The point is a solution. Q.E.D.

In the case of a single source in D, the explicit form of the solution to optimal control problem (8.3) is given by Theorem 3.

Theorem 3. *Let $Q(t)$ be the strength of a point source located at the point $\mathbf{r}_0$ and let $J(\psi_{\vec{Q}}) > J_0$. Then*

$$\begin{aligned} Q^*(t) &= Q(t) - \beta g(\mathbf{r}_0, t), \\ \beta &= \{J(\psi_Q) - J_0\} / \int_0^T g^2(\mathbf{r}_0, t) dt \quad (8.6) \end{aligned}$$

is a solution of problem (8.3), if $Q^*(t) \geq 0$ for all $t \in [0, T]$.

Proof. Consider the Lagrangian

$$L(q) = F(q) - \mathcal{G} \left(\int_0^T g(\mathbf{r}_0, t) q(t) dt - \alpha \right)$$

The solution (8.6) is its first variation. In fact, $Q^*(t)$ is positive and belongs to Θ , because

$$\begin{aligned} &\int_0^T g(\mathbf{r}_0, t) Q^*(t) dt \\ &= J_0 - \int_D g(\mathbf{r}, 0) \psi^0(\mathbf{r}) d\mathbf{r} = \alpha \end{aligned}$$

Let $q(t) = Q^*(t) + \delta q(t)$ belong to the set Θ and differ from $Q^*(t)$. Then

$$\begin{aligned} &-\int_0^T g(\mathbf{r}_0, t) \delta q(t) dt \\ &\geq \int_0^T g(\mathbf{r}_0, t) Q^*(t) dt - \alpha \end{aligned}$$

and

$$\begin{aligned} F(q) - F(Q^*) &= -2\beta \int_0^T g(\mathbf{r}_0, t) \delta q(t) dt \\ &+ \int_0^T [\delta q(t)]^2 dt > 0 \end{aligned}$$

Consequently, (8.6) is a solution to problem (8.3). Q.E.D.

9 Identification of intensity of a new point source

Estimating the intensity of an unknown air pollution source based on a given set of observed data is a classical inverse problem.

Addressing these issues is of particular importance in view of efforts to determine fault of individuals and enterprises and to assess environmental impacts.

Since the problem (1.1)-(1.6) is linear, we assume that only a single source is active, located at point

$\mathbf{r}_0 \in D$, $\psi^0(\mathbf{r}) \equiv 0$ and its emission rate $Q(t)$ is unknown.

Let $\mathbf{R} \in D$ be the monitoring place, and let $\psi(\mathbf{R}, t_j)$ denote the pollutant concentration calculated using the dispersion model at the place $\mathbf{R}$ and time $t_j \in (0, T)$, $j = 1, 2, \dots, M$. Then the adjoint estimate (6.6) of the pollutant concentration $\psi(\mathbf{R}, t_j)$ is

$$\psi(\mathbf{R}, t_j) = \int_0^{t_j} Q(t) g_j(\mathbf{r}_0, t) dt, \\ j = 1, 2, \dots, M \quad (9.1)$$

In (9.1), we considered that the adjoint model solution $g_j(\mathbf{r}, t)$ is equal to zero on the interval (t_j, T) . Therefore, for each j , the solution $g_j(\mathbf{r}, t)$ of the adjoint problem (5.1)-(5.4) must be calculated only in the time interval $(0, t_j)$ under the condition $g_j(\mathbf{r}, t_j) = 0$, $\mathbf{r} \in D$. These adjoint solutions depends only on the dispersion conditions, the monitoring site $\mathbf{R}$, the moment of sampling t_j , but are independent of the source intensity $Q(t)$. Relations (9.1) describe the explicit relationship between the emission level $Q(t)$ (cause) and the pollutant concentration $\psi(\mathbf{R}, t_j)$ at point $\mathbf{R}$ and time t_j (effect). It should be noted that to use equations (9.1) it is necessary to calculate M different solutions of the adjoint problem (5.1)-(5.4).

In the particular case when the process of atmospheric dispersion is stationary, the operator of the dispersion problem does not depend on time. Therefore,

$$g_j(\mathbf{r}, t) = g_\alpha(\mathbf{r}, T - t_j + t) \text{ in } (0, t_j), \\ j = 1, 2, \dots, M \quad (9.2)$$

where g_α , called the basic kernel, is the solution to the adjoint problem (5.1)-(5.4) for $p(\mathbf{r}, t) = \delta(t - T)\delta(\mathbf{r} - \mathbf{R})$. The use of basic kernel simplifies the calculations, since formulas (9.1) take the form

$$\psi(\mathbf{R}, t_j) = \int_0^{t_j} Q(t) g_\alpha(\mathbf{r}_0, T - t_j + t) dt, \\ j = 1, 2, \dots, M \quad (9.3)$$

and by calculating only kernel g_α one can establish explicit connections between $Q(t)$ and $\psi(\mathbf{R}, t_j)$.

Assume that the measurements at the place $\mathbf{R}$ contain minor errors $\delta\psi_j$,

$$\psi_j(\mathbf{R}) = \psi(\mathbf{R}, t_j) + \delta\psi_j, \\ j = 1, 2, \dots, M \quad (9.4)$$

with the mean error equal to zero:

$$\frac{1}{M} \sum_{j=1}^M \delta\psi_j = 0 \quad (9.5)$$

9.1 Unknown constant source

Suppose that a pollutant source with unknown constant intensity $Q(t) = Q_c$ acts in $t \in (0, T)$ at a known point $\mathbf{r}_0 \in D$.

Then relations (9.1) take the form

$$\psi(\mathbf{R}, t_j) = Q_c \int_0^{t_j} g_j(\mathbf{r}_0, t) dt, \\ j = 1, 2, \dots, M \quad (9.6)$$

Summing relations (9.6) over j from 1 to M and using (9.5) we obtain

$$\sum_{j=1}^M \psi(\mathbf{R}, t_j) = Q_c \sum_{j=1}^M \int_0^{t_j} g_j(\mathbf{r}_0, t) dt \quad (9.7)$$

Due to (9.4) and (9.5),

$$\sum_{j=1}^M \psi_j(\mathbf{R}) = \sum_{j=1}^M \psi(\mathbf{R}, t_j),$$

and (9.7) leads to

$$\sum_{j=1}^M \psi_j(\mathbf{R}) = Q_c \sum_{j=1}^M \int_0^{t_j} g_j(\mathbf{r}_0, t) dt$$

Therefore,

$$Q_c = \left\{ \sum_{j=1}^M \psi_j(\mathbf{R}) \right\} \left\{ \sum_{j=1}^M \int_0^{t_j} g_j(\mathbf{r}_0, t) dt \right\}^{-1} \quad (9.8)$$

Thus, measurements $\psi_j(\mathbf{R})$ and pollutant concentrations $\psi(\mathbf{R}, t_j)$ calculated using the dispersion model, allow to determine the constant intensity of the source if its location $\mathbf{r}_0$ is known.

9.2 Unknown instantaneous source

Let us assume that at a specific (known) time t_e^* and at a specific (known) point $\mathbf{r}_0$, an instantaneous release of a pollutant of unknown intensity Q_e occurred, - that is,

$$Q(t) = Q_e \delta(t - t_e^*), \quad 0 < t_e^* < T \quad (9.9)$$

Therefore, due to (9.1),

$$\begin{aligned}\psi(\mathbf{R}, t_j) &= Q_e \int_0^{t_j} \delta(t - t_e^*) g_j(\mathbf{r}_0, t) dt \\ &= Q_e g_j(\mathbf{r}_0, t_e^*), \quad j = 1, 2, \dots, M \quad (9.10)\end{aligned}$$

Summing relations (9.10) over j again, and using equations (9.4), (9.5), we get

$$Q_e = \left(\sum_{j=1}^M \psi_j(\mathbf{R}) \right) \left\{ \sum_{j=1}^M g_j(\mathbf{r}_0, t_e^*) \right\}^{-1} \quad (9.11)$$

9.3 The total mass of a pollutant emitted from a non-stationary source

Estimation of the emission level of an unknown nonstationary point source it is more complicated. However, it is easy to estimate the minimum of the total mass of the pollutant emitted into the atmosphere as a result of the accident. Such an assessment can be performed if the location $\mathbf{r}_0$ of the source is known. A recent example is the release of radioactive substances from the Fukushima nuclear power plant [9]. In what follows, we denote by

$$m = \int_0^T Q(t) dt$$

the total mass of a pollutant released from a source located at point $\mathbf{r}_0$ within the time $(0, T)$.

Definition 2. A monitoring site $\mathbf{R}$ will be called *useful* if

$$\sum_{j=1}^M \psi_j(\mathbf{R}) > 0$$

for the time series $\{\psi_j(\mathbf{R})\}_{j=1}^M$.

Definition 3. Let $\mathbf{R}$ be a useful monitoring site. We denote

$$\psi_R = \sum_{j=1}^M \psi_j(\mathbf{R}) \quad \text{and} \quad \hat{g}_R(t) = \sum_{j=1}^M g_j(\mathbf{r}_0, t)$$

Theorem 4. Let $\mathbf{R}_1, \dots, \mathbf{R}_N$ be useful monitoring sites. Then

$$m \geq \max_{1 \leq i \leq N} \left\{ \psi_{R_i} / G_{R_i} \right\}$$

where

$$\begin{aligned}G_{R_i} &= \max_{0 \leq t \leq T} \left\{ \hat{g}_{R_i}(t) \right\} > 0 \\ i &= 1, \dots, N \quad (9.12)\end{aligned}$$

Proof. We assume that condition (9.5) is satisfied. Then, summing relations (9.1) over all j , substituting equations (9.4) and (9.5) into the sum, and considering Definition 3, we get

$$\psi_{R_i} = \int_0^T Q(t) \hat{g}_{R_i}(t) dt, \quad i = 1, \dots, N$$

By definition of G_{R_i} , we have

$$\int_0^T Q(t) \hat{g}_{R_i}(t) dt \leq G_{R_i} \int_0^T Q(t) dt, \quad i = 1, \dots, N,$$

and therefore

$$\frac{\psi_{R_i}}{G_{R_i}} \leq \int_0^T Q(t) dt, \quad i = 1, \dots, N.$$

Applying the maximum to this inequality over all i , we estimate the minimum for the total mass m . Q.E.D.

9.4 Average intensity of a non-stationary source

Let $Q(t)$ be an unknown emission level $Q(t)$ of the point source. Assume we know its location $\mathbf{r}_0$ in the region D . Let us denote by $\bar{Q}$ the average intensity of this source during a time interval $(0, T)$. To estimate $\bar{Q}$ of this source we sum formula (9.1) over index j , use (9.4), (9.5), and apply the mean value theorem. As a result,

$$\begin{aligned}\sum_{j=1}^M \psi_j(\mathbf{R}) &= \sum_{j=1}^M \psi(\mathbf{R}, t_j) = \sum_{j=1}^M \int_0^T Q(t) g_j(\mathbf{r}_0, t) dt \\ &= \int_0^T Q(t) \left\{ \sum_{j=1}^M g_j(\mathbf{r}_0, t) \right\} dt = \bar{Q} \sum_{j=1}^M \int_0^T g_j(\mathbf{r}_0, t) dt\end{aligned}$$

and

$$\bar{Q} = \left\{ \sum_{j=1}^M \psi_j(\mathbf{R}) \right\} \left\{ \sum_{j=1}^M \int_0^T g_j(\mathbf{r}_0, t) dt \right\}^{-1}$$

(9.13)

It should be noted that all the results obtained for the case where condition (9.5) holds can be generalized to the case

$$\left(\sum_{j=1}^M \delta \psi_j \right) / M \neq 0.$$

10 Identification of the location of permanent and instantaneous sources

In Section 9, assuming the source location $\mathbf{r}_0$ to be known, we determined the unknown discharge levels Q_c and Q_e for constant and instantaneous sources. In this Section, we propose a method for identifying the location $\mathbf{r}_0$ of a continuous source, as well as the location $\mathbf{r}_0$ and time of release t_e of an instantaneous

source. We will introduce nonlinear Localization Functions whose zeros will define both $\mathbf{r}_0$ and t_e^* . After determining these two parameters, the emission rates of both sources are determined by formulas (9.8) and (9.11).

10.1 Constant source

Assume that the emission rate of the source is constant: $Q(t) = Q_c = \text{Const}$, $t \in (0, T)$.

Definition 4. For useful monitoring site $\mathbf{R}$ we define

$$\psi_R = \sum_{j=1}^M \psi_j \quad \text{and} \quad \hat{g}_R(\mathbf{r}) = \int_0^T \left\{ \sum_{j=1}^M g_j(\mathbf{r}, t) \right\} dt$$

Theorem 5. If $\mathbf{R}, \mathbf{R}_1, \dots, \mathbf{R}_N$ are useful monitoring sites then the source location $\mathbf{r}_0$ is the zero of the Localization Function

$$\Phi(\mathbf{r}) = \ln \left\{ 1 + \sum_{i=1}^N [\psi_R \hat{g}_{R_i}(\mathbf{r}) - \psi_{R_i} \hat{g}_R(\mathbf{r})]^2 \right\} \quad (10.1)$$

while the discharge rate is

$$Q_c = \psi_R \{\hat{g}_R(\mathbf{r}_0)\}^{-1}.$$

Proof. Application of (9.8) to each site yields

$$Q_c = \frac{\psi_R}{\hat{g}_R(\mathbf{r}_0)}$$

and

$$Q_c = \frac{\psi_{R_i}}{\hat{g}_{R_i}(\mathbf{r}_0)}, \quad i = 1, \dots, N$$

Then

$$\frac{\psi_{R_i}}{\hat{g}_{R_i}(\mathbf{r}_0)} = \frac{\psi_R}{\hat{g}_R(\mathbf{r}_0)}, \quad \text{or}$$

$$(\psi_R \hat{g}_{R_i}(\mathbf{r}_0) - \psi_{R_i} \hat{g}_R(\mathbf{r}_0))^2 = 0, \quad i = 1, \dots, N$$

Summing over i yields

$$\sum_{i=1}^N [\psi_R \hat{g}_{R_i}(\mathbf{r}_0) - \psi_{R_i} \hat{g}_R(\mathbf{r}_0)]^2 = 0 \quad (10.2)$$

i.e., $\Phi(\mathbf{r}_0) = 0$. Once the source position $\mathbf{r}_0$ is determined, the source intensity Q_c is calculated using formula (9.8). Q.E.D.

10.2 Instantaneous source

For an instantaneous source (9.9), it is necessary to determine three parameters: the location $\mathbf{r}_0$ and

strength Q_e of the source as well as the release time t_e^* .

Definition 5. For useful monitoring site $\mathbf{R}$ we define

$$\psi_R = \sum_{j=1}^M \psi_j \quad \text{and} \quad \hat{g}_R(\mathbf{r}, t_e) = \sum_{j=1}^M g_j(\mathbf{r}, t_e).$$

Theorem 6. If $\mathbf{R}, \mathbf{R}_1, \dots, \mathbf{R}_N$ are useful monitoring site then the point $(\mathbf{r}_0, t_e^*)$ is the zero of the Localization Function

$$\Phi(\mathbf{r}, t_e) = \ln \left\{ 1 + \sum_{i=1}^N [\psi_R \hat{g}_{R_i}(\mathbf{r}, t_e) - \psi_{R_i} \hat{g}_R(\mathbf{r}, t_e)]^2 \right\} \quad (10.3)$$

while the discharge rate is

$$Q_e = \hat{\phi}_R / \hat{g}_R(\mathbf{r}_0, t_e^*).$$

Proof. Application of (9.11) to each site yields

$$Q_e = \frac{\psi_R}{\hat{g}_R(\mathbf{r}_0, t_e^*)} \quad \text{and} \quad Q_e = \frac{\psi_{R_i}}{\hat{g}_{R_i}(\mathbf{r}_0, t_e^*)}, \quad i = 1, \dots, N$$

Then

$$\frac{\psi_{R_i}}{\hat{g}_{R_i}(\mathbf{r}_0, t_e^*)} = \frac{\psi_R}{\hat{g}_R(\mathbf{r}_0, t_e^*)}, \quad \text{or}$$

$$(\psi_R \hat{g}_{R_i}(\mathbf{r}_0, t_e^*) - \psi_{R_i} \hat{g}_R(\mathbf{r}_0, t_e^*))^2 = 0, \quad i = 1, \dots, N$$

Summing over i yields

$$\sum_{i=1}^N (\psi_R \hat{g}_{R_i}(\mathbf{r}_0, t_e^*) - \psi_{R_i} \hat{g}_R(\mathbf{r}_0, t_e^*))^2 = 0 \quad (10.4)$$

From (10.4) it follows that $\Phi(\mathbf{r}_0, t_e^*) = 0$. After finding $\mathbf{r}_0$ and t_e^* from $\Phi(\mathbf{r}_0, t_e^*) = 0$, Q_e is determined using formula (9.11). Q.E.D.

Note that the functions $\hat{g}_R$ are positive. Therefore, the admissible set for $\mathbf{R}_i$ is

$$F_c = \left\{ \mathbf{r}_0 \in D : \prod_{i=1}^N \hat{g}_{R_i}(\mathbf{r}_0) > 0 \right\} \quad (10.5)$$

for the constant source, and

$$F_e = \left\{ (\mathbf{r}_0, t_e) \in D \times (0, T) : \prod_{i=1}^N \hat{g}_{R_i}(\mathbf{r}_0, t_e) > 0 \right\}$$

(10.6)

for the instantaneous source. In practice, knowledge of the admissible regions (10.5) and (10.6) narrows the search range for the zeros of Localization Functions and lowers computational overhead.

11 Tikhonov regularization for the identification of nonstationary outliers

Assume that the point source intensity depends on time, and

$$\psi_j(\mathbf{R}) = \psi(\mathbf{R}, t_j) + \delta\psi_j, \quad j = 1, 2, \dots, M$$

at the site $\mathbf{R}$. We now present a method for reconstructing nonstationary discharge rates. Consider the following inverse problem:

$$\text{minimize } J(Q) = \frac{1}{2} \int_0^T \left(\frac{dQ}{dt} \right)^2 dt \quad (11.1)$$

$$\text{subject to } Q(t) \geq 0, \quad t \in (0, T),$$

$$Q(0) = Q(T) = 0 \quad (11.2)$$

and

$$-\varepsilon \leq \psi_j(\mathbf{R}) - \int_0^{t_j} Q(t) g_j(\mathbf{r}_0, t) dt \leq \varepsilon, \quad j = 1, \dots, M \quad (11.3)$$

This problem is solved using the Tikhonov regularization method. The functional (11.1) is minimized to filter out errors $\delta\psi_j$ and determine the magnitude of outliers. The parameter $\varepsilon > 0$ is used to expand the feasible region of the inverse problem. This parameter influences the solution smoothness, and its optimum value coincides with the maximum error magnitude $\delta\psi_j$.

11.1 Existence and uniqueness of a regularized solution

We now prove the existence and uniqueness of a regularized solution of problem (11.1)-(11.3) [8]. Let H be the Hilbert space of real-valued absolutely continuous functions on $[0, T]$ such that $q(0) = q(T) = 0$ and $q'(t) \equiv \partial q / \partial t$ is square integrable. The inner product and norm in H are defined as follows:

$$(p, q)_H = \int_0^T p'(t) q'(t) dt, \quad (11.4)$$

$$\|q\|_H = \sqrt{(q, q)_H}.$$

The unknown discharge level $Q(t) \in H$, since it is a non-negative continuously differentiable function, i.e., $Q(t) \in C^1[0, T]$ and $Q(0) = Q(T) = 0$.

The feasible set for the variational problem (11.1)-(11.3) is defined as

$$F_\varepsilon = \{q \in H : q(t) \geq 0 \text{ in } [0, T] \text{ and}$$

$$-\varepsilon \leq \psi_j(\mathbf{R}) - \int_0^{t_j} q(t) g_j(\mathbf{r}_0, t) dt \leq \varepsilon, \quad j = 1, \dots, M \quad (11.5)$$

where

$$\varepsilon \geq \varepsilon^* = \max_j |\delta\psi_j|.$$

Due to (9.5), $Q \in F_\varepsilon$ for all $\varepsilon \geq \varepsilon^*$, and consequently F_ε is a non-empty set in the space H . We now need some results to prove the existence and uniqueness of the regularized solution to the inverse problem.

Theorem 7 [1]. *A non-empty closed convex set in a uniformly convex Banach space has a unique point closest to a given point.*

Lemma 3 [1]. *The space H is a uniformly convex Banach space.*

Lemma 4. *The feasible space F_ε is a convex set in H .*

Proof. Let $q_1, q_2 \in F_\varepsilon$ and $\lambda \in (0, 1)$. Then $\lambda q_1 + (1 - \lambda)q_2 \in H$ and $\lambda q_1 + (1 - \lambda)q_2 \geq 0$ in $[0, T]$. However, for each j ($j = 1, \dots, M$), we have

$$\begin{aligned} & \left| \psi_j(\mathbf{R}) - \int_0^{t_j} [\lambda q_1(t) + (1 - \lambda)q_2(t)] g_j(\mathbf{r}_0, t) dt \right| \\ & \leq \lambda \left| \psi_j(\mathbf{R}) - \int_0^{t_j} q_1(t) g_j(\mathbf{r}_0, t) dt \right| \\ & \quad + (1 - \lambda) \left| \psi_j(\mathbf{R}) - \int_0^{t_j} q_2(t) g_j(\mathbf{r}_0, t) dt \right| \\ & \leq \lambda \varepsilon + (1 - \lambda) \varepsilon = \varepsilon \end{aligned}$$

Thus, $\lambda q_1 + (1 - \lambda)q_2 \in F_\varepsilon$ and F_ε is convex. Q.E.D.

Lemma 5. *Any sequence converging in the space H converges uniformly.*

Proof. Let $q(t) \in H$. Then

$$\begin{aligned} 2|q(t)| &= \left| \int_0^t q'(\tau) d\tau - \int_t^T q'(\tau) d\tau \right| \\ &= \left| \int_0^t \text{sgn}(t - \tau) q'(\tau) d\tau + \int_t^T \text{sgn}(t - \tau) q'(\tau) d\tau \right| \\ &= \left| \int_0^T \text{sgn}(t - \tau) q'(\tau) d\tau \right| \end{aligned}$$

where $t \in [0, T]$. Therefore, using the Schwarz inequality, we obtain

$$2|q(t)| \leq \sqrt{\int_0^T [\text{sgn}(t - \tau)]^2 d\tau} \|q\|_H = \sqrt{T} \|q\|_H \quad (11.6)$$

As a result, any converging in H sequence converges uniformly. Q.E.D.

Lemma 6. The feasible space F_ε is a closed set in H .

Proof. We now demonstrate that $\bar{F}_\varepsilon \subset F_\varepsilon$. Let $q \in \bar{F}_\varepsilon$. Then, there is a sequence $\{q_n\}_{n=1}^\infty$ in F_ε such that $\|q_n - q\|_H \rightarrow 0$ as $n \rightarrow \infty$, and according to Lemma 5, $\{q_n\}$ converges to q uniformly. Moreover,

$$\begin{aligned} & \left| \psi_j(\mathbf{R}) - \int_0^{t_j} q(t) g_j(\mathbf{r}_0, t) dt \right| \\ &= \left| \psi_j(\mathbf{R}) - \int_0^T q(t) g_j(\mathbf{r}_0, t) dt \right| \\ &\leq \left| \psi_j(\mathbf{R}) - \int_0^T q_n(t) g_j(\mathbf{r}_0, t) dt \right| \\ &\quad + \int_0^T |q(t) - q_n(t)| g_j(\mathbf{r}_0, t) dt \end{aligned}$$

Let

$$C = \max_j \int_0^T g_j(\mathbf{r}_0, t) dt < \infty.$$

Using (11.3) and (11.6) in the last estimate leads to

$$\begin{aligned} & \left| \psi_j(\mathbf{R}) - \int_0^{t_j} q(t) g_j(\mathbf{r}_0, t) dt \right| \\ &\leq \varepsilon + 0.5\sqrt{T} \|q - q_n\|_H \int_0^T g_j(\mathbf{r}_0, t) dt \\ &\leq \varepsilon + 0.5C\sqrt{T} \|q - q_n\|_H \end{aligned}$$

and

$$\left| \psi_j(\mathbf{R}) - \int_0^{t_j} q(t) g_j(\mathbf{r}_0, t) dt \right| \leq \varepsilon$$

as $n \rightarrow \infty$. Thus, all constraints in (11.5) are satisfied.

The inequality $q(t) \geq 0$ is demonstrated using the law of contradiction. Let $q(t_0) < 0$ for some $t_0 \in (0, T)$.

Due to uniform convergence of the sequence $\{q_n\}$ to q on $[0, T]$ as $n \rightarrow \infty$,

$$|q_N(t_0) - q(t_0)| < |q(t_0)|/2$$

for sufficiently large number N , and therefore

$$q_N(t_0) < q(t_0)/2 < 0,$$

which contradicts the fact that $q_N \in F_\varepsilon$. Thus, $q \in F_\varepsilon$. Q.E.D.

Note that $q_c(t) \equiv 0$ is the only constant function in the space H , besides, due to Lemma 7, $q_c(t) \notin F_\varepsilon$.

Thus, the regularized solution Q_ε to the inverse problem can be neither zero nor constant.

Lemma 7. If $\psi_K(\mathbf{R}) > \varepsilon^* = \max_j |\delta\psi_j|$ for some K ($1 \leq K \leq M$) then $q_c \notin F_\varepsilon$ for any ε from the interval $\varepsilon^* \leq \varepsilon < \psi_K(\mathbf{R})$.

Proof. Let us apply the law of contradiction once again. If $q_c \in F_\varepsilon$ then

$$\psi_K(\mathbf{R}) - \int_0^{t_K} q_c g_K(\mathbf{r}_0, t) dt \leq \varepsilon$$

for some K in (11.5), i.e., $\psi_K(\mathbf{R}) \leq \varepsilon$ which contradicts $\varepsilon < \psi_K(\mathbf{R})$, and consequently $q_c \notin F_\varepsilon$. Q.E.D.

It should be noted that the condition $\psi_K(\mathbf{R}) > \varepsilon^*$ is fully justified and implies that the values $\psi(\mathbf{R}, t_j)$ significantly exceed the data uncertainties.

Theorem 8. Let $\psi_K(\mathbf{R}) > \varepsilon^* = \max_j |\delta\psi_j|$ for some K ($1 \leq K \leq M$). Then the variational problem (11.1)-(11.3) has a unique non-trivial solution for any $\varepsilon \in [\varepsilon^*, \psi_K(\mathbf{R}))$.

Proof. By Lemma 3, H is a uniformly convex Banach space, and by virtue of (9.4), $Q \in F_\varepsilon$ for all $\varepsilon \geq \varepsilon^*$, i.e., F_ε is a non-empty set. In addition, according to Lemmas 4 and 6, the feasible space F_ε is a closed convex set in H . Note that $q_c \notin F_\varepsilon$ as $\varepsilon < \psi_K(\mathbf{R})$. As a result, by Theorem 7, there is a unique function Q_ε in the feasible space F_ε that minimizes the distance to the function q_c . By virtue of (11.1), Q_ε also minimizes the functional $J(q)$ on the feasible space F_ε . Therefore, Q_ε is a regularized solution of the inverse problem.

12 Numerical experiments

Let us consider a 1D pollution model:

$$\begin{aligned} \frac{\partial \psi}{\partial t} - \mu \frac{\partial^2 \psi}{\partial x^2} + \sigma \psi &= Q(t) \delta(x - x_0), \\ x &\in (0, 1), t \in (0, T) \end{aligned} \quad (12.1)$$

$$\mu \frac{\partial \psi}{\partial x}(0, t) = 0, \quad t > 0 \quad (12.2)$$

$$\mu \frac{\partial \psi}{\partial x}(1, t) = -\zeta \psi(1, t), \quad t > 0 \quad (12.3)$$

$$\psi(x, 0) = 0 \quad x \in (0, 1) \quad (12.4)$$

where $\mu > 0$ and $\sigma \geq 0$, x_0 is the source location in $D = (0, 1)$, and $Q(t)$ is the source intensity. As a result, the pollutant mass in D increases because of

intensity Q and decreases owing to outflow at $x = 1$ and exponential decrease ($\sigma > 0$):

$$\frac{\partial}{\partial t} \int_0^1 \psi(x, t) dx = Q(t) - \zeta \psi(1, t) - \int_0^1 \sigma \psi(x, t) dt$$

The problem operator

$$A = -\mu \frac{\partial^2 \psi}{\partial x^2} + \sigma \psi$$

is positive semidefinite:

$$(A\psi, \psi) = \int_0^1 \mu \left(\frac{\partial \psi}{\partial x} \right)^2 dx + \zeta \psi^2(1, t) + \int_0^1 \sigma \psi^2(x, t) dt \geq 0$$

Consequently, the well posed diffusion model (12.1) - (12.4) exists, is unique, and depends continuously on the initial condition and the external driver.

Applying Lagrange's identity $(A\psi, g) = (\psi, A^*g)$ to the problem (12.1) - (12.4) makes it possible to desing the following adjoint problem:

$$-\frac{\partial g_j}{\partial t} - \mu \frac{\partial^2 g_j}{\partial x^2} + \sigma g_j = p(x, t), \\ x \in (0, 1), t \in (0, T) \quad (12.5)$$

$$\mu \frac{\partial g_j}{\partial x}(0, t) = 0, t > 0 \quad (12.6)$$

$$\mu \frac{\partial g_j}{\partial x}(1, t) = -\zeta g_j(1, t), t > 0 \quad (12.7)$$

$$g_j(x, T) = 0, x \in (0, 1) \quad (12.8)$$

Where $p(x, t) = \delta(t - t_j)\delta(x - \mathbf{R})$ is the forcing, and $\mathbf{R}$ is the monitoring site in D . As a result, we obtain

$$\psi(\mathbf{R}, t_j) = \int_0^{t_j} Q(t) g_j(x_0, t) dt$$

We now use dispersion model (12.1) - (12.4) to estimate the parameters of constant and instantaneous sources. Since the dispersion conditions in this example are stationary, the basic kernel

$$g_\alpha(x_0, t) = \sum_{k=1}^{\infty} c_k e^{-(\lambda_k^2 \mu + \sigma)(T-t)} \cos(\lambda_k x_0), \\ t \in (0, T) \quad (12.9)$$

has the property $g_\alpha(x_0, T - t_j + t) = g_j(x_0, t)$ for $t \leq t_j$. Thus, the solutions g_j of the adjoint model (12.5) - (12.8) are calculated using the basic kernel (12.9). Figure 2 shows the basic kernel $g_\alpha(x_0, t)$ and

adjoint functions $g_j(x_0, t)$ for the moments $t_j = 3$ and $t_j = 15$. For series (12.9), the following parameters were used: $x_0 = 0.5 \text{ km}$, $\mathbf{R} = 0.2 \text{ km}$, $\zeta = 1.0 \text{ km}$, $\mu = 0.1 \text{ km}^2$, $\sigma = 0.01 \text{ h}^{-1}$, $T = 20 \text{ h}$ and $K = 10000$.

Synthetic data ψ_j are generated according to equation (9.4), where the corresponding values $\psi(\mathbf{R}, t_j)$ for each experiment are calculated using the Fejér-Fourier series, and the errors $\delta\psi_j$ are uniformly distributed with zero mean value.

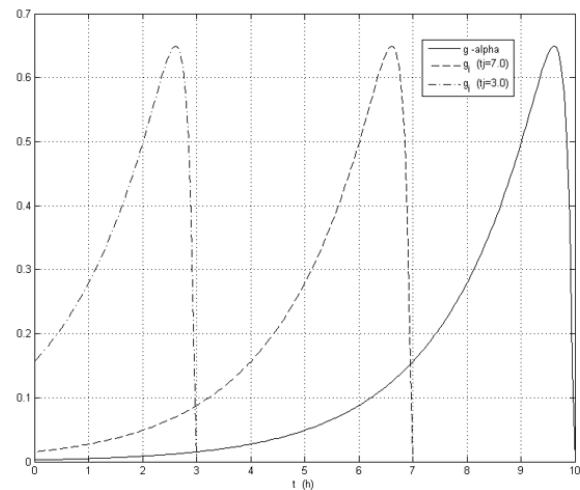


Fig. 2. Basic kernel $g_\alpha(x_0, t)$ and adjoint functions $g_j(x_0, t)$ for $t_j = 3$ and $t_j = 15$.

Experiment 1. First, consider a constant source located at the point $x_0^* = 0.5 \text{ km}$ with intensity $Q_c = 100 \text{ kg h}^{-1}$. Figure 3, Figure 4 and Figure 5 show the Localization Function $\Phi(x_0)$ for different monitoring areas $\mathbf{R}$ and $\mathbf{R}_1$. It should be noted that in all cases, the zero of the Localization Functions $\Phi(x_0)$ correctly determine the location of the emission source. In addition, Theorem 5 allows us to correctly calculate the intensity $Q_c = 100$ of the source.

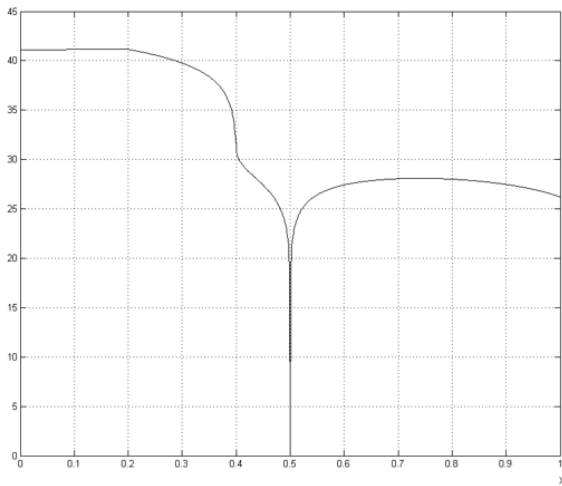


Fig. 3. Localization Function $\Phi(x_0)$ for the monitoring sites $R = 0.2$ and $R_1 = 0.4$.

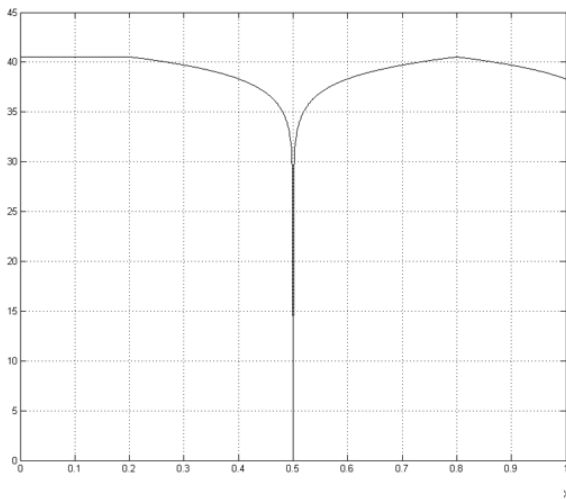


Fig. 4. Localization Function $\Phi(x_0)$ for the monitoring sites $R = 0.2$ and $R_1 = 0.8$.

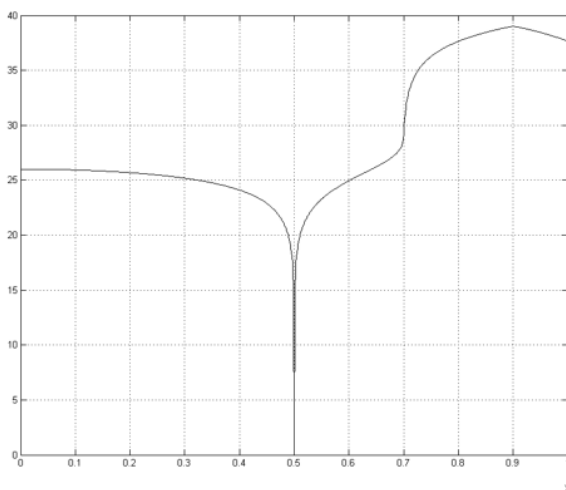


Fig. 5. Localization Function $\Phi(x_0)$ for the monitoring sites $R = 0.7$ and $R_1 = 0.9$.

Experiment 2. Let us consider the case of an instantaneous source located at $x_0^* = 0.7 \text{ km}$ with a strength $Q_e = 120 \text{ kg}$ at time $t_e^* = 12 \text{ h}$. Figure 6 and Figure 7 show Localization Functions $\Phi(x_0, t_e)$ for various monitoring sites R and R_1 .

We see that the zeros of Localization Functions correctly identify the place and moment of the emission. Furthermore, Theorem 8 makes it possible to correctly calculate the source strength $Q_e = 120$.

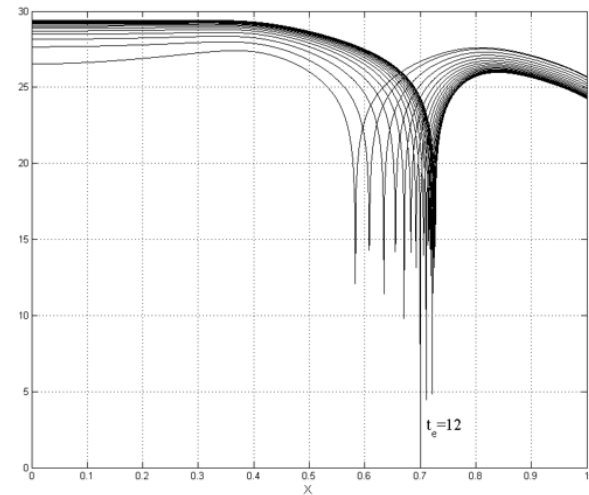


Fig. 6. Cross-sections of the Localization Function $\Phi(x_0, t_e)$ for different t_e . The monitoring sites are $R = 0.4$ and $R_1 = 0.8$.

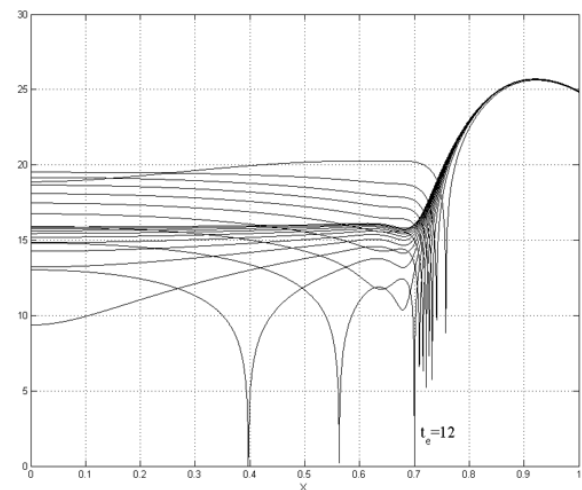


Fig. 7. Cross-sections of the Localization Function $\Phi(x_0, t_e)$ for different t_e . The monitoring sites are $R = 0.8$ and $R_1 = 0.9$.

Compliance with Ethical Standards

The authors thank National System of Researcher of Mexico (Sistema Nacional de Investigadores de México, CONACYT) for supporting their research through fellowships 14539 and 25170 over the years.

Declaration of Generative AI and AI-assisted Technologies in the Writing Process

During the preparation of this work, the author(s) utilized artificial intelligence (AI) technologies solely for the purpose of linguistic refinement and grammatical correction. Following the application of these tools, the author(s) comprehensively reviewed, verified, and edited the resulting text. The author(s) maintain full accountability and responsibility for the accuracy, integrity, and final content of the publication.

References:

- [1] Cheney E.W. (1966). Introduction to Approximation Theory. Chelsea, New York.
- [2] Godunov S.K. (1971). Equations of Mathematical Physics. Nauka, Moscow.
- [3] Hadamard J. (1923). Lectures on Cauchy's Problem in Linear Partial Differential Equations. Yale University Press, New Haven, CT.
- [4] Marchuk G.I. (1986). Mathematical Models in Environmental Problems. North-Holland, Amsterdam.
- [5] Marchuk G.I. and Yu.N. Skiba (1976). Numerical calculation of the conjugate problem for a model of the thermal interaction of the atmosphere with the oceans and continents, *Izv., Atmos. Ocean. Phys.* 12 (5), 279-284.
- [6] Parra-Guevara D. and Yu.N. Skiba (2003). Elements of the mathematical modelling in the control of pollutants emissions. *Ecological Modelling* 167 (3), 263-275.
- [7] Parra-Guevara, D. and Yu.N. Skiba (2006). On optimal solution of an inverse air pollution problem: theory and numerical approach. *Math. Comput. Model.* 43 (7-8), 766-778.
- [8] Parra-Guevara D., Yu.N. Skiba and A. Reyes-Romero (2014). Existence and uniqueness of the regularized solution in the problem of recovery the non-steady emission rate of a point source: Application of the adjoint method. In: *Engineering Optimization IV – Rodrigues et al. (Eds.)*, CRC Press 2014, London, pp. 181-186.

- [9] Sharma L.K., A.K. Ghosh, R.N. Nair, M. Chopra, F. Sunny and V.D. Puranik (2014). Inverse modeling for aquatic source and transport parameters identification and its application to Fukushima nuclear accident. *Environ. Model. Assess.* 19, 193-206.
- [10] Skiba, Yu.N. and D. Parra-Guevara (2024). Mathematical methods for the assessment and control of industrial emissions. Springer Nature AG, Cham, Switzerland. <https://doi.org/10.1007/978-3-031-58109-0>.

Contribution of individual authors to the creation of a scientific article (ghostwriting policy)

All authors (Yuri N. Skiba and David Parra-Guevara) contributed to the development of this paper. Conceptualisation, All authors; Methodology, All authors; Analytical and Numerical Analysis, All authors; Validation, All authors; Writing-original draft preparation, All authors; Writing-review and editing, All authors.

Sources of Funding for Research Presented in a Scientific Article or Scientific Article Itself

No funding was received for conducting this study.

Conflict of Interest

The authors have no conflicts of interest to declare that are relevant to the content of this study.

Creative Commons Attribution License 4.0 (Attribution 4.0 International, CC BY 4.0)

This article is published under the terms of the Creative Commons Attribution License 4.0 https://creativecommons.org/licenses/by/4.0/deed.en_US