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Air quality short-term control in an industrial region under adverse weather conditions

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Abstract

A new short-term optimal control of air quality in an industrial region during atmospheric inversions is proposed. Its goal is to prevent violation of health standard of air quality in a few monitored zones. The control establishes restrictions on the emission rates of industrial sources and includes the identification of the industrial sources violating (exceeding) the emission rates set by the control. Both control and identification are based on using solutions to an adjoint dispersion model. Conditions that show the convergence of the emission rates, prescribed by the control, to the original emission rates of the industrial sources are given (Theorems 4 and 5). These results ensure that the new emission rates of industrial sources (established by the control) will be as close as possible to the original emission rates throughout the entire period of application of the control. This creates the minimum possible restrictions on the functioning of industrial enterprises. The highlight of the new control is the possibility of selecting special weights for each pollution source in the goal function that is minimized. These weights are mainly aimed at reducing the intensity of emissions of the main sources of pollution. An example demonstrates the ability of the new method. A similar approach can also be used to develop methods for cleaning water zones polluted by oil (the problem of bioremediation), and to prevent excessive pollution of urban areas with automobile emissions.

Keywords: Dispersion model, adjoint model, adjoint estimates, optimal control, source detection

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1 Introduction

The purpose of this study is to propose a new mathematical method for protecting the air quality in an industrial region during adverse weather conditions. The method is the optimal short-term control of emission rates of industrial sources. In the case when a dispersion model predicts an excess of the maximum permissible concentration of a pollutant in a monitored zone, the control determines new, optimal to some extent, emission rates for the industrial sources. From this point on, each industrial source should continue its work with

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reduced emission rates prescribed by the control. This prevents a violation of the air quality standard in the monitored zones selected in the industrial region. In the case of constant emission rates, a method of identifying the industrial sources that exceed the emission rates set by the control is also given. Both methods are based on using a dispersion model and its adjoint model. The highlight of the new control is the possibility of selecting special weights for each pollution source in the goal function that is minimized. These weights are aimed at reducing the intensity of emissions of those sources that pollute the most. Conditions that show the convergence of the emission rates, prescribed by the control, to the original emission rates of the industrial sources are given (Theorems 4 and 5). These results ensure that the reduced emission rates of industrial sources (established by the control) will be as close as possible to the original emission rates throughout the entire period of application of the control. This creates the minimum possible restrictions on the functioning of industrial enterprises.

The new control can be applied to dispersion models of various degrees of complexity. In this work, we use a two-dimensional (vertically integrated) dispersion model in a limited area with open boundaries whose unique solvability was proved in [1]. It is easy to justify the use of such model during atmospheric inversions. Indeed, the intensity of emissions of pollution sources should usually be reduced under adverse meteorological conditions, when dispersion of pollutants is difficult and, above all, when an inversion layer forms on the Earth's surface. In meteorology, an inversion is almost always a deviation from the normal change of the air temperature with altitude. Usually the air at the surface of the Earth is warmer than the air above it, that is, the air temperature decreases with altitude. Under an atmospheric inversion, warmer air is held above cooler air, i.e., the normal temperature profile with altitude is inverted. The height of the inversion layer of air can reach hundreds of meters, and therefore high pipes of industrial enterprises cannot save the situation. Inversion detains contaminants close to the ground, preventing them from dispersing, and all contaminants accumulate in the inversion layer, covering the industrial region until the meteorological conditions change. This phenomenon creates the greatest danger to human health. An inversion also suppresses convection (vertical movements) by acting as a "cap". Under such conditions the use of two-dimensional (vertically integrated within the inversion layer) model can give satisfactory results.

Also, to simplify the analysis, we assume that the wind velocity is known from a model of atmospheric dynamics or from observations (using, for example, monthly mean climatic wind velocities), and therefore the dispersion model contains only the advection-diffusion equation. Of course, in practice, the combination of the control strategy with a more realistic dispersion model will give a better result.

An adjoint dispersion model is introduced using the Lagrange identity and the definition of adjoint operator [2]. Then dual (direct and adjoint) estimates of the pollution concentration are derived in a few ecologically most sensitive areas (monitored zones). The adjoint estimates depend explicitly on the number of the sources, their positions and emission rates, as well as on the initial distribution of pollutant in the region. In these estimates, the solutions to adjoint problems serve as weighting functions that determine the contribution of each industrial source to the pollution of a selected monitored zone. Therefore, adjoint estimates play an important role in studying the sensitivity of the dispersion model to changes in its parameters and in developing optimal short-term control of industrial emissions under adverse weather conditions.

The control can be applied whenever a dispersion model gives an unsatisfactory air quality forecast. It prescribes to reduce the emission rate of each industrial source in advance to avoid violating the air quality standards in the monitored zones the next day (days).

Note that optimal control strategies can be distinguished from each other by the goal functions that need to be minimized. An example is given to show the skilfull of the proposed control strategy. The work ends with a description of the method of identification of industrial sources that exceed the emission rates established by the control.

2 Dispersion model in a limited area

Let D be a two-dimensional limited area with open boundary S. Assume that there are N industrial sources located at points $\boldsymbol{r}_i = (x_i, y_i)$ of domain D, which operate with emission rates $Q_i(t)$, $0 < t < T$, $i = 1, 2, \ldots, N$. Let $\phi(\boldsymbol{r}, t)$ denote the concentration of a pollutant at a point $\boldsymbol{r} = (x, y)$ of domain D and time t. The dispersion model in the domain D and time interval $(0, T)$ is

$$\frac{\partial}{\partial t}\phi + A\phi = f(\boldsymbol{r}, t), \tag{1}$$

where

$$A\phi = \mathrm{div}(\boldsymbol{U}\phi) + \sigma\phi - \mathrm{div}(\mu\,\nabla\phi) \tag{2}$$

and $\boldsymbol{U}(\boldsymbol{r}, t) = \{u(\boldsymbol{r}, t), v(\boldsymbol{r}, t)\}$ is a known wind velocity that satisfies the continuity equation

$$\mathrm{div}\boldsymbol{U} = 0. \tag{3}$$

The term $\sigma\phi$ describes an exponential decay of $\phi(\boldsymbol{r}, t)$ due to physical and chemical processes ($\sigma(\boldsymbol{r}, t) > 0$), $\mu(\boldsymbol{r}, t) > 0$ is the coefficient of turbulent diffusion,

$$f(\boldsymbol{r}, t) \equiv \sum_{i=1}^{N} Q_i(t)\delta(\boldsymbol{r} - \boldsymbol{r}_i) \tag{4}$$

is the pollution forcing, and $\delta(\boldsymbol{r} - \boldsymbol{r}_i)$ is the Dirac delta function. As the initial condition we take

$$\phi(\boldsymbol{r}, 0) = \phi^0(\boldsymbol{r}) \text{ at } t = 0, \tag{5}$$

where $\phi^0(\boldsymbol{r})$ is the known initial distribution of the pollutant concentration in D.

Usually the pollution flux through the open boundary S of domain D is unknown, and any errors in the pollution flux at the boundary perturb the solution inside D. Therefore, it is important to put such boundary conditions that guaranty the existence, uniqueness and stability of the model solution in space-time domain $D \times (0, T)$. In this work, we take the boundary conditions supposed in [1] under which the problem is well posed both physically and mathematically:

$$\mu\frac{\partial}{\partial n}\phi = 0 \text{ at } S^+;\ \mu\frac{\partial}{\partial n}\phi - U_n\phi = 0 \text{ at } S^-. \tag{6}$$

In conditions (6), $U_n = \boldsymbol{U} \cdot \boldsymbol{n}$ is the projection of velocity $\boldsymbol{U}$ on the unit external normal $\boldsymbol{n}$ to the boundary S, and the boundary $S = S^+ \cup S^-$ is divided into the "inflow" part S^- (where $U_n < 0$, i.e., the pollution flux is directed inside D) and "outflow" part S^+ (where $U_n \geqslant 0$, and the pollution flux is directed outside D) (Fig. 1). Operator (2) is positively semidefinite [3], and therefore problem (1)–(6) is well posed according to Hadamard [4], namely, it has a unique solution $\phi(\boldsymbol{r}, t)$ that continuously depends on the initial distribution $\phi^0(\boldsymbol{r})$, the number of sources N, their positions $\boldsymbol{r}_i$ and emission rates $Q_i(t)$.

The total mass of pollutant in D is $\int_D \phi \mathrm{d}\boldsymbol{r}$, and we consider value $\|\phi(\boldsymbol{r}, t)\| = (\int_D \phi^2 \mathrm{d}\boldsymbol{r})^{\frac{1}{2}}$ as the norm of the solution. It is easy to see that these values obey the integral equations

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_D \phi\,\mathrm{d}\boldsymbol{r} = \sum_{i=1}^{N} Q_i(t) - \int_D \sigma\phi\,\mathrm{d}\boldsymbol{r} - \int_{S^+} U_n\phi \mathrm{d}S, \tag{7}$$

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_D \phi^2 \mathrm{d}\boldsymbol{r} = 2\sum_{i=1}^{N} Q_i(t)\phi(\boldsymbol{r}_i, t) - 2\int_D (\sigma\phi^2 + \mu|\nabla\phi|^2)\mathrm{d}\boldsymbol{r} - \int_S |U_n|\phi^2 \mathrm{d}S. \tag{8}$$

Thus, the total mass of pollutant in D and the norm of solution to problem (1)–(6) increase due to nonzero emission rates $Q_i(t)$, and decrease due to dissipative processes ($\sigma > 0, \mu > 0$) and outflow of pollutant through the part S^+ of the boundary. If $f(\boldsymbol{r}, t) \equiv 0$ (industrial activity in the region is stopped), the dissipative processes are neglected ($\sigma = 0, \mu = 0$) and $U_n = 0$ everywhere at the boundary S (there is no flow of pollutants through the boundary), then both integrals are conserved:

$$\int_D \phi \mathrm{d}\boldsymbol{r} = \text{const} \text{ and } \int_D \phi^2 \mathrm{d}\boldsymbol{r} = \text{const}. \tag{9}$$

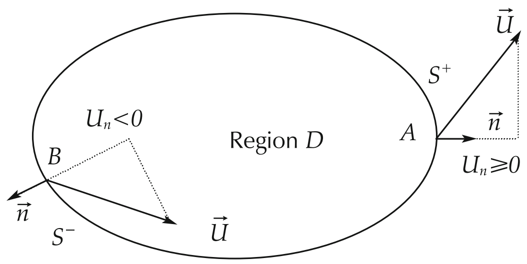

Fig. 1 Open boundary $S = S^+ \cup S^-$ of domain D. Point A belongs to S^+, and point B belongs to S^-.

Despite the obvious artificiality of the condition $U_n = 0$ at the open boundary S, the equations (7)–(9) are useful in testing numerical algorithms and computational programs.

3 Adjoint model

Obviously, the solution $\phi(\boldsymbol{r}, t)$ of problem (1)–(6) determines the concentration of pollutant at any point of the space-time domain $D \times (0, T)$. Suppose now that we want to know the contribution of each industrial source to the pollution of some ecologically sensitive monitored zone Ω located in domain D. To this end, problem (1)–(6) must be solved N times, separately for each source of pollution. And if the number N of industrial sources is large then this approach will require considerable computation. In this case, using the dispersion model (1)–(6) is not the optimal way, and the contribution of each source is much easier to determine using the so-called *adjoint estimates* based on the use of the solutions to an adjoint dispersion model [5]. These solutions serve as valuable information functions [6].

Thus, in addition to the model (1)–(6), we consider in the space-time domain $D \times (0, T)$ the adjoint model

$$-\frac{\partial g}{\partial t} + A^* g = p(\boldsymbol{r}, t), \tag{10}$$

where $\boldsymbol{U}(\boldsymbol{r}, t) = \{u(\boldsymbol{r}, t), v(\boldsymbol{r}, t)\}$ is the wind velocity of the dispersion model, and

$$A^* g = -\mathrm{div}(\boldsymbol{U} g) + \sigma g - \mathrm{div}(\mu \nabla g). \tag{11}$$

At the inflow and outflow parts of boundary S the adjoint model has the following conditions:

$$\mu \frac{\partial g}{\partial n} + U_n g = 0 \ \text{ at } \ S^+; \ \ \mu \frac{\partial g}{\partial n} = 0 \ \text{ at } \ S^-. \tag{12}$$

As the "initial" condition for the adjoint problem we take

$$g(\boldsymbol{r}, T) = 0 \ \text{ at } \ t = T \ \text{ in } \ D \tag{13}$$

because this problem is well posed only if solved from $t = T$ to $t = 0$. Note that the wind velocity $\boldsymbol{U}(\boldsymbol{r}, t)$ and coefficients $\mu(\boldsymbol{r}, t)$ and $\sigma(\boldsymbol{r}, t)$ in the adjoint model are the same as in the dispersion model (1)–(6), while forcing $p(\boldsymbol{r}, t)$ is still undefined. Thus,

$$\mathrm{div} \boldsymbol{U} = 0. \tag{14}$$

How is the adjoint model constructed? This is briefly explained in Appendix A.

4 Direct and adjoint estimates

Let us define the mean concentration of pollutant $\phi(\boldsymbol{r}, t)$ in the ecologically sensitive zone $\Omega \subset D$ and time interval $(T - \tau, T)$ as

$$J(\phi) = \frac{1}{\tau |\Omega|} \int_{T-\tau}^{T} \int_{\Omega} \phi(\boldsymbol{r}, t) \mathrm{d}\boldsymbol{r} \mathrm{d}t. \tag{15}$$

We will call (15) *direct estimate* of mean concentration of $\phi(\boldsymbol{r}, t)$ in Ω. It requires to solve the dispersion model (1)–(6). We will now derive one more estimate of value (15) using the solution to adjoint model (10)–(13).

A combination of problems (1)–(6) and (10)–(13) on the base of Lagrange identity, integration in time from 0 to T, and the use of conditions (5) and (12) leads to

$$\begin{aligned} &\int_0^T \mathrm{d}t \int_D p(\boldsymbol{r}, t) \phi(\boldsymbol{r}, t) \mathrm{d}\boldsymbol{r} \\ &= \int_0^T \mathrm{d}t \int_D g(\boldsymbol{r}, t) f(\boldsymbol{r}, t) \mathrm{d}\boldsymbol{r} + \int_D g(\boldsymbol{r}, 0) \phi^0(\boldsymbol{r}) \mathrm{d}\boldsymbol{r}. \end{aligned} \tag{16}$$

Let us define forcing $p(\boldsymbol{r}, t)$ in (10) as

$$p(\boldsymbol{r}, t) = \begin{cases} \dfrac{1}{\tau |\Omega|}, & \text{if } (\boldsymbol{r}, t) \in \Omega \times (T - \tau, T), \\ 0, & \text{otherwise.} \end{cases}$$

Then substituting (4) and such determined $p(\boldsymbol{r}, t)$ in (16) we obtain

$$J(\phi) = \sum_{i=1}^{N} \int_0^T g(\boldsymbol{r}_i, t) Q_i(t) \mathrm{d}t + \int_D g(\boldsymbol{r}, 0) \phi^0(\boldsymbol{r}) \mathrm{d}\boldsymbol{r}. \tag{17}$$

It is so-called *adjoint estimate* of mean concentration of $\phi(\boldsymbol{r}, t)$ in Ω. It is equivalent to (15). However, unlike (15), estimate (17) is independent of the solution $\phi(\boldsymbol{r}, t)$ of dispersion problem (1)–(6) and uses only values $g(\boldsymbol{r}_i, t)$ and $g(\boldsymbol{r}, 0)$ of the adjoint model solution at positions $\boldsymbol{r}_i$ of industrial sources and at $t = 0$, respectively.

The last integral in (17) which determines the contribution of initial pollution in D we denote it as

$$c_0 = \int_D g(\boldsymbol{r}, 0) \, \phi^0(\boldsymbol{r}) \mathrm{d}\boldsymbol{r}. \tag{18}$$

The dual estimates (15) and (17) complement each other depending on the situation. The direct estimate (15) uses the solution $\phi(\boldsymbol{r}, t)$ of dispersion problem (1)–(6), and hence, this problem must be solved again whenever the number N of sources, their positions $\boldsymbol{r}_i$ and emission rates $Q_i(t)$ vary. Thus, the direct estimates should be used if the pollution concentration is evaluated at each point, or in many zones of domain D. However, such comprehensive information is rather costly and often unnecessary. In many cases it is sufficient to know value (15) only in few ecologically most important zones of region D. Then it is much simpler to find the solution $g(\boldsymbol{r}, t)$ of the adjoint model (10)–(13) for each zone Ω and use the adjoint estimate (17). Sometimes they give an immediate solution to non-trivial problems [7–10].

It should be emphasized that the adjoint estimates play an important role in controlling emission rates of pollution sources. In contrast to (1)–(6), the adjoint problem (10)–(13) is independent on the number of sources N, their positions $\boldsymbol{r}_i$ and emission rates $Q_i(t)$, and therefore its solution can be found for each zone Ω independently of specific values of all these parameters.

5 Optimal short-term control of emission rates

Let a forecast model M (in our case, the model (1)–(5)) is used to predict the concentration $\phi_{\vec{Q}}(\boldsymbol{r},t)$ of a pollutant in the domain D and time interval $(-t_0, T)$ using the emission rates $\vec{Q}(t) = \{Q_1(t), \dots, Q_N(t)\}$ of N industrial sources emitting a pollutant. Here $t_0 > 0$ is the time required to fulfill the forecast in the interval $(-t_0, T)$ and control in the interval $(0, T)$ (see Fig. 2). Suppose that the forecast is unsatisfactory in the sense that

$$J(\phi_{\vec{Q}}) > J_0, \tag{19}$$

i.e., the mean concentration of the pollutant in a monitored zone $\Omega \subset D$ and time interval $(T-\tau, T)$ exceeds the air quality standard J_0 (see (17) and Fig. 2). Therefore, the goal of control is to determine in the interval $(0, T)$ such reduced emission rates $\vec{q}(t) = \{q_1(t), \dots, q_N(t)\}$ of industrial sources that

$$J(\phi_{\vec{q}}) \leqslant J_0 \tag{20}$$

in $\Omega \times (T-\tau, T)$. Let

$$F(\vec{q}) = \frac{1}{2}\sum_{i=1}^{N} \gamma_i^2 \|Q_i - q_i\|^2 = \frac{1}{2}\sum_{i=1}^{N} \gamma_i^2 \int_0^T (Q_i - q_i)^2 \mathrm{d}t \tag{21}$$

be defined in the domain

$$\Theta = \{\vec{q}(t) : q_i(t) \geqslant 0, i = 1, 2, \dots, N;\ J(\phi_{\vec{q}}) \leqslant J_0\}. \tag{22}$$

Thus, Θ is the set of such emission rates $\vec{q}(t) = \{q_1(t), \dots, q_N(t)\}$ that guarantee the compliance with the air quality standard J_0 in Ω: $J(\phi) \leqslant J_0$.

The optimal control consists in finding such rates $\vec{Q}^*(t) \in \Theta$ that minimize the function $F(\vec{q})$ in the feasible set Θ:

$$F(\vec{Q}^*) = \min\{F(\vec{q}) : \vec{q} \in \Theta\}. \tag{23}$$

Clearly, the control depends on the norm $\|\cdot\|$ used in (21). In this work we use the norm in the space $L_2(0, T)$. Note that $\vec{Q}^*(t)$ is the optimal solution that represents the least restriction on the work of industrial sources (i.e., the new emission rates $\vec{Q}^*(t)$ are as close to the original emission rates $\vec{Q}(t)$ as possible).

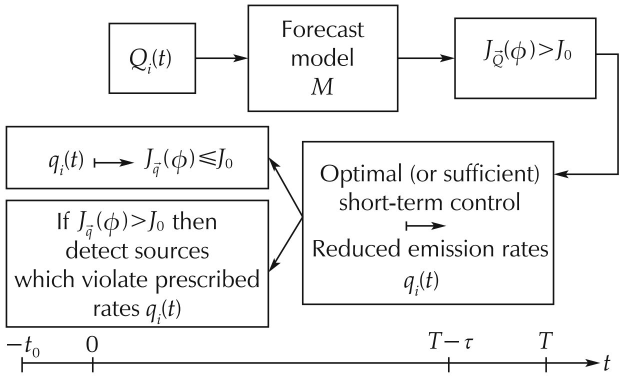

Fig. 2 Scheme of a short-term control within time interval $(0, T)$.

The weights $\gamma_i, i = 1, 2, \dots, N$ for the objective function (21) will be selected as follows. Let

$$c_i = \int_0^T g(\boldsymbol{r}_i, t) Q_i(t) \mathrm{d}t > 0$$

denote the mean concentration obtained in the monitored zone Ω only due to emissions from the ith pollution source ($i = 1, 2, \dots, N$). Then $f_i = \dfrac{c_i}{c_1 + \dots + c_N}$ is the portion of pollution produced by the ith source, and we select $\gamma_i = \dfrac{1}{f_i}$. Thus, γ_i tends to be large for a small portion of f_i. For each monitored zone Ω, c_i and γ_i can be calculated by using the adjoint model solution and formula (17). Each weight γ_i introduced in (21) is in favor of small polluters. Indeed, each pollution source with a lower impact in the monitored zone Ω gets a larger weight γ_i. As a result, the control sets the optimal emission rate $Q_i^*(t)$ for this source closer to the original one $Q_i(t)$. Thus, formulas (21)–(23) represent a new control of emissions from industrial sources, which is primarily aimed at reducing emission rates of major sources of pollution. For explaining the role of weights γ_i in (21) let us consider a simple example of optimization problem.

Example 1 Suppose that $c_0 = 0$ (see (18)) and there are only two industrial sources in the region D. Then the optimal control is

$$\min \to F = \frac{1}{2}[\gamma_1^2(Q_1 - q_1)^2 + \gamma_2^2(Q_2 - q_2)^2]$$
$$\text{subject to } \beta_1 q_1 + \beta_2 q_2 = J_0,\ \beta_1 \neq 0,\ \beta_2 \neq 0.$$

We used here the first mean value theorem for definite integrals

$$\int_0^T g(\boldsymbol{r}_i, t)q_i(t)\mathrm{d}t = q_i \int_0^T g(\boldsymbol{r}_i, t)\mathrm{d}t = \beta_i q_i, \quad i = 1, 2,$$

where $g(\boldsymbol{r}_i, t)$ is the value of the adjoint solution at the position $\boldsymbol{r}_i$ of the ith industrial source. The optimal solution that minimizes F is expressed as

$$Q_2^* = Q_2\Big(\frac{1}{\big(\frac{\gamma_1}{\gamma_2}\big)^2\big(\frac{\beta_2}{\beta_1}\big)^2 + 1}\Big) + \beta_2\Big(\frac{J_0 - \beta_1 Q_1}{\beta_2^2 + \big(\frac{\gamma_2}{\gamma_1}\big)^2\beta_1^2}\Big),$$
$$Q_1^* = \frac{J_0 - \beta_2 Q_2^*}{\beta_1}.$$

It is easy seen that $Q_2^* \to Q_2$ as $\gamma_2 \to \infty$. On the other way, if $\gamma_1 \to \infty$ then $Q_2^* \to \dfrac{J_0 - \beta_1 Q_1}{\beta_2}$, and due to the second equation,

$$Q_1^* = \frac{J_0 - \beta_2 Q_2^*}{\beta_1}, \ \text{ i.e., } \ Q_1^* \to Q_1.$$

Note that the variational problem (23) can be solved by an iterative optimization method using a consistent evaluation of the dynamic model M. Usually, this process is not very efficient because it may require many calculations due to the complexity of model M. Therefore, let us now propose an alternative method based on the use of the adjoint operator, which allows us to solve the problem of optimal control without a successive evaluation of the dynamic model.

The solution to problem (23) is critically dependent on the parameter

$$\alpha = J_0 - \int_D g(\boldsymbol{r}, 0)\,\phi^0(\boldsymbol{r})\mathrm{d}\boldsymbol{r}.$$

Indeed, for $\alpha < 0$ there is no solution to (23) because the sanitary norm will not be maintained even if all emissions are reduced to zero (i.e., any production activity in the domain D will be stopped).

The following two theorems are valid for any selection of the positive weights γ_i in (21). They can be proved in the same way as in [11].

Theorem 1 Let $\alpha = 0$. Then the optimal control problem (23) has only one solution

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

where $I_i = \{t \in [0, T] : g(\boldsymbol{r}_i, t) > 0\}$, $1 \leqslant i \leqslant N$.

Theorem 2 If $\alpha > 0$ then the optimal control problem (23) has a unique solution $\vec{Q}^* \in \Theta$ such that $Q_i^*(t) \leqslant Q_i(t)$ $(0 \leqslant t \leqslant T, \ 1 \leqslant i \leqslant N)$ and $J(\phi) = J_0$.

If there is only one source in the region, the statement of Theorem 2 can be specified:

Theorem 3 Suppose that there is only one industrial source with emission rate $Q(t)$ located at the point $\boldsymbol{r}_1$ of the domain D. If $\alpha > 0$ and $J(\phi) > J_0$ then

$$\begin{cases} Q^*(t) = Q(t) - \beta g(\boldsymbol{r}_1, t), \\ \beta = \dfrac{J(\phi) - J_0}{\int_0^T g^2(\boldsymbol{r}_1, t)\mathrm{d}t} \end{cases} \tag{24}$$

is the only solution to the optimal control (23), provided that $Q^*(t) \geqslant 0$ for any $t \in [0, T]$.

By Theorem 2, the feasible set (22) reduces to a much smaller set

$$\Theta = \{q_i(t) \geqslant 0 : \sum_{i=1}^N \int_0^T g(\boldsymbol{r}_i, t)q_i(t)\mathrm{d}t = \alpha\}. \tag{25}$$

An approximate (numerical) solution to the problem of optimal control is obtained with highly effective numerical algorithm of sequential orthogonal projections [11]. From the computational view point, the new set Θ is much less than (22), and therefore preferable in calculations.

Remark 1 We will show in Appendix B that equation (24) also suggests a non-optimal strategy to control the emission rates. For this, we define new emission rates $\hat{Q}_i(t)$, $i = 1, 2, \dots, N$, as follows:

$$\hat{Q}_i(t) = Q_i(t) - \beta_i g(\boldsymbol{r}_i, t),$$
$$\beta_i = \frac{c_i + (c_0 - J_0)f_i}{\int_0^T g^2(\boldsymbol{r}_i, t)\mathrm{d}t},$$

where $c_0 = \int_D g(\boldsymbol{r}, 0)\phi^0(\boldsymbol{r})\mathrm{d}\boldsymbol{r}$ and $c_i = \int_0^T g(\boldsymbol{r}_i, t)Q_i(t)\mathrm{d}t$.

6 Convergence of emission rates prescribed by the control

The following two assertions give the conditions under which the emission rates prescribed by the controls $\hat{Q}_i(t)$ and $Q_i^*(t)$ converge to the original emission rates of industrial sources.

Theorem 4 Suppose that for all i and $t \in (0, T)$

$$\frac{Q_i(t)}{\|Q_i\|} \geqslant \frac{J(\phi_{\vec{Q}}) - J_0}{J(\phi_{\vec{Q}}) - c_0} \frac{g(\boldsymbol{r}_i, t)}{\|g(\boldsymbol{r}_i, t)\|}. \tag{26}$$

Then $\hat{Q}_i(t) \geqslant 0$ for all i and $t \in (0, T)$. Besides, $\hat{Q}_i \to Q_i$ uniformly on $(0, T)$ as $J(\phi_{\vec{Q}}) \to J_0$.

The proof of this theorem is given in Appendix C. Theorem 4 assures that if the excess over the sanitary norm, $J(\phi_{\vec{Q}}) - J_0$, is small then for all moments, the temporal behavior of rates $\hat{Q}_i(t)$ prescribed by the control will approximate the temporal behavior of the original emission rates $Q_i(t)$. In other words, no major changes in the work of industrial sources are required. Note that such control is obtained directly from the adjoint functions.

The following theorem characterizes the convergence of the optimal rates Q_i^*.

Theorem 5 Suppose that the condition (26) is satisfied. Then, for all i,

$$\|Q_i - Q_i^*\|^2 \leqslant \Big(\frac{J(\phi_{\vec{Q}}) - J_0}{\gamma_i}\Big)^2 \sum_{j=1}^{N} \frac{1}{\|g(\boldsymbol{r}_j, t)\|^2}. \tag{27}$$

Therefore, $\|Q_i - Q_i^*\| \to 0$ as $\gamma_i \to \infty$ or when $J(\phi_{\vec{Q}}) \to J_0$.

The proof of this theorem is given in Appendix D. Theorems 4 and 5 show the convergence of the new emission rates, established by the controls, to the original emission rates of the industrial sources. These results ensure that the new emission rates of industrial sources will be as close as possible to the original emission rates throughout the entire period of application of the control. This creates the minimum possible restrictions on the functioning of industrial enterprises.

7 Optimal short-term control with synthetic data

To demonstrate the capabilities of the new control strategy, we now consider a numerical example using synthetic data. The six industrial sources are considered in the domain $D = (0, 5) \times (0, 5)$, and the control of emissions is applied in the time interval $(0, T)$ where $T = 8$. As a monitored zone we take $\Omega = (2, 3) \times (2, 3)$ during the whole interval, i.e., $\tau = T = 8$. Fig. 3 shows the location $\boldsymbol{r}_i$ of the point sources ($i = 1, 2, \ldots, 6$), the position of zone Ω, and the nondivergent wind velocity $\boldsymbol{U} = (u, v)$ where $u(x, y) = y^2/25$ and $v(x, y) = x/5$. The diffusion and transformation parameters for the dispersion model are $\mu = 0.1$ and $\sigma = 0.001$, respectively.

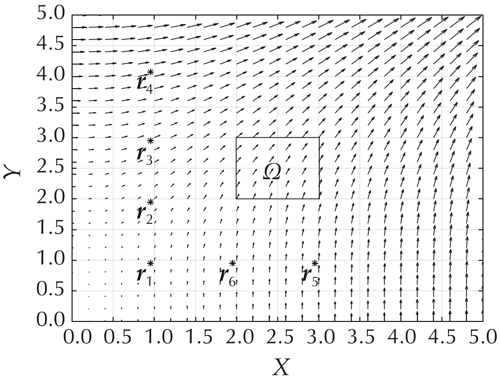

Fig. 3 The location $\boldsymbol{r}_i$ of the point sources and monitored zone Ω in domain D. The arrows show the wind direction $\boldsymbol{U}$.

The emission rates of the six industrial sources during the interval $(0, T)$ are as follows:

$$Q_1(t) = 3,\ \ Q_2(t) = 10e^{-(t-4)^2},$$
$$Q_3(t) = |t-2|,\ \ Q_4(t) = 2 - 0.5\cos(\frac{\pi}{2}t),$$
$$Q_5(t) = 2e^{-(t-1)^2} \ \text{and}\ \ Q_6(t) = e^{-(t-3)^2} + 2e^{-(t-5)^2}.$$

In this example, the initial distribution of the pollutant at $t = 0$ is taken uniform and small: $\phi(\boldsymbol{r}, 0) = 0.2$. Due to the work of sources and initial condition, the mean concentration of pollutant $J(\phi_{\vec{Q}})$ in the monitored zone Ω is 1.7596 and exceeds the sanitary standard $J_0 = 1.5$ [12]. Then the optimal control method is used to reduce the emission rates and respect the sanitary standard J_0.

At the first stage, the adjoint problem is solved backward from $t = T$ to $t = 0$. Figs. 4 and 5 show the isolines of the adjoint function $g(\boldsymbol{r}, t)$ in D, at $t = 6$ and $t = 4$. It is seen that the area of nonzero values of $g(\boldsymbol{r}, t)$ expands in the southwestern direction, opposite to the direction of the wind speed in D, as it must be. Therefore, the focus should be on monitoring the emission rates of sources located in the south-western part of the domain D.

Using the adjoint solution $g(\boldsymbol{r}, t)$, one can estimate the pollution levels c_i in the monitored zone. The values c_i, f_i and γ_i for each point source are contained in Table 1. Besides, in our case, $c_0 = 0.1391$ and $\alpha = J_0 - c_0 = 1.3609 > 0$. According to fractions f_i, the sources located at points $\boldsymbol{r}_3$ and $\boldsymbol{r}_4$ make an insignificant contribution to the pollution of zone Ω. Therefore, it is expected that the optimal control will prescribe minimal reductions in their emission rates. Figs. 6–11 show the original emission rates Q_i and the optimal rates Q_i^* for each source.

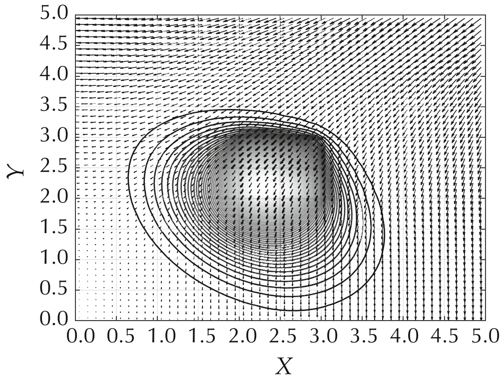

Fig. 4 Isolines of the adjoint function $g(\boldsymbol{r}, t)$ at $t = 6$.

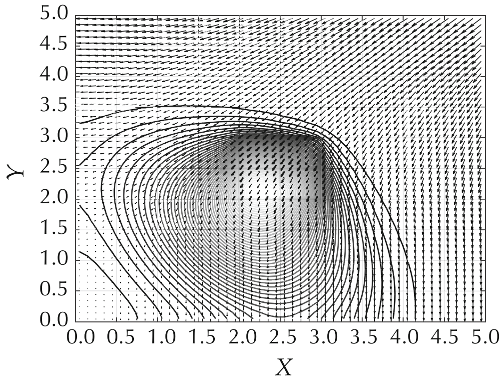

Fig. 5 Isolines of the adjoint function $g(\boldsymbol{r}, t)$ at $t = 4$.

Table 1 Location $\boldsymbol{r}_i$ and coefficients c_i, f_i and γ_i of each pollution source.

i	$\boldsymbol{r}_i$	c_i	f_i	γ_i
1	(0.95,0.95)	0.4785	0.2953	3.3867
2	(0.95,1.95)	0.5286	0.3262	3.0654
3	(0.95,2.95)	0.1212	0.0748	13.3660
4	(0.95,3.95)	0.0082	0.0051	196.6810
5	(2.95,0.95)	0.1992	0.1230	8.1330
6	(1.95,0.95)	0.2846	0.1757	5.6931

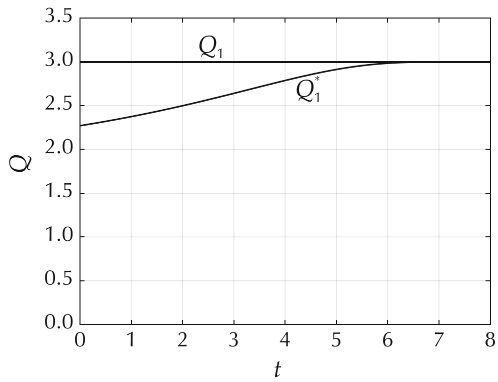

Fig. 6 The emission rate $Q_1(t)$ and the optimal rate $Q_1^*(t)$ in time interval $(0, T)$.

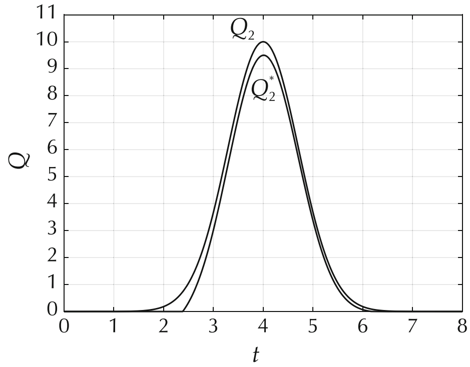

Fig. 7 The emission rate $Q_2(t)$ and the optimal rate $Q_2^*(t)$ in time interval $(0, T)$.

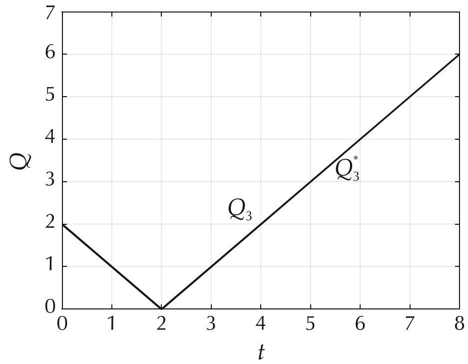

Fig. 8 The emission rate $Q_3(t)$ and the optimal rate $Q_3^*(t)$ in time interval $(0, T)$.

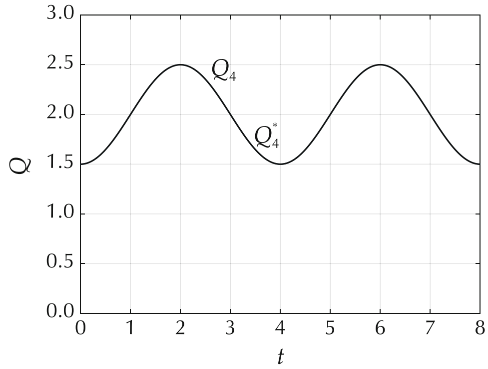

Fig. 9 The emission rate $Q_4(t)$ and the optimal rate $Q_4^*(t)$ in time interval $(0, T)$.

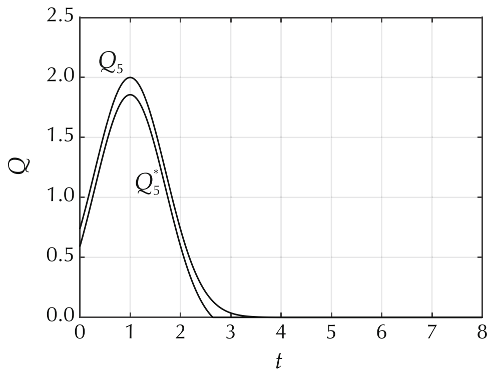

Fig. 10 The emission rate $Q_5(t)$ and the optimal rate $Q_5^*(t)$ in time interval $(0, T)$.

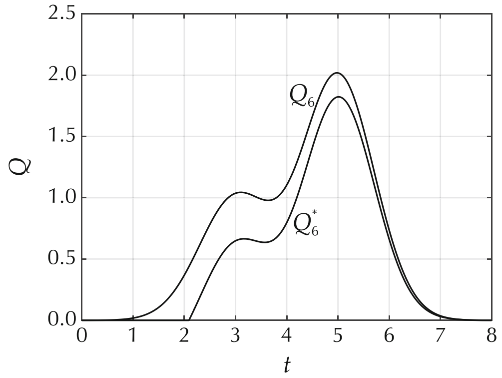

Fig. 11 The emission rate $Q_6(t)$ and the optimal rate $Q_6^*(t)$ in time interval $(0, T)$.

Figs. 8 and 9 show that the original and optimal emission rates of the sources, located at points $\boldsymbol{r}_3$ and $\boldsymbol{r}_4$, are almost equal. Finally, we point out that the CPU-time used to find the numerical solution of the adjoint model [13], together with the optimal emission rates for this example is less than 2 min.

8 Detection of the sources which exceed prescribed emissions

In practice, there are the situations when, despite of applying a control strategy, the measurements show the violation of air quality standard again: $J(\phi) > J_0$. It means that some industrial sources exceed the emission rates $q_i(t)$ prescribed by the control, and are responsible for excessively polluting the zone Ω. We now briefly describe a way to detect such sources.

Let $Q_i(t)$ be original emission rates of industrial sources, and let $q_i(t)$ be reduced emission rates prescribed by a control in order to satisfy the air quality standard in $\Omega \times (T-\tau, T)$: $J(\phi) \leqslant J_0$. Suppose that some sources ignored this requirement and continued to work with unknown emission rates $\bar{Q}_i(t) > q_i(t)$, and hence are responsible for excessively polluting the zone Ω. This raises the question of detection and sanctioning of such sources. Though the detection problem is not trivial for time-dependent emission rates, it can easily be solved for invariable emission rates. Note that the assumption of stationary emission rates is not a strong limitation if the time interval $(0, T)$ is sufficiently small [14].

Suppose that in the interval $(0, T)$, the i*th* industry had to operate at a constant emission rate q_i, prescribed by the control, but it worked at an unknown constant rate $\bar{Q}_i$. Let $\delta Q_i = Q_i - \bar{Q}_i$ $(i = 1, 2, \dots, N)$, and let $J(\phi)$ and $\bar{J}(\phi)$ be the mean pollutant concentrations (15) in the zone Ω predicted by the model before control and measured after control, respectively. Thus,

$$\delta J(\phi) = J(\phi) - \bar{J}(\phi) \tag{28}$$

is a known value. Let us choose K zones in the domain D $(K \geqslant N)$, and denote as $\delta J_k(\phi)$ the value (28) obtained for the kth zone Ω_k $(k = 1, 2, \dots, K)$. Denote the solution to adjoint problem (10)–(13) for the zone Ω_k by $g_k(\boldsymbol{r}, t)$, and its value at the position $\boldsymbol{r}_i$ of the ith industry by $g_k(\boldsymbol{r}_i, t)$ $(i = 1, 2, \dots, N)$. Taking into account that in our case, $\delta\phi^0(\boldsymbol{r}) \equiv 0$, and δQ_i is constant for each i, the adjoint estimates (17) for K zones lead to a linear system

$$\sum_{i=1}^{N} a_{ki} \delta Q_i = \delta J_k(\phi), \quad k = 1, 2, \dots, K \tag{29}$$

with non-negative elements

$$a_{ik} = \int_0^T g_k(\boldsymbol{r}_i, t) \mathrm{d}t \tag{30}$$

of the $N \times K$ matrix $(i = 1, 2, \dots, N;\ k = 1, 2, \dots, K)$. If $K > N$ then matrix is rectangular and system $A\vec{x} = \vec{b}$ given by (29) and (30) can be solved by the method of least squares: $\vec{x} = (A^{\mathrm{T}}A)^{-1}A^{\mathrm{T}}\vec{b}$. Solution to (29) gives the values δQ_i, and hence, the values $\bar{Q}_i = Q_i - \delta Q_i$. Thus, if for some i, $\bar{Q}_i > q_i$ then the ith plant violated the prescribed emission rate in the interval $(0, T)$.

9 Conclusions

A new mathematical method for protecting the air quality in an industrial region during adverse weather conditions is proposed. For the case of constant emission rates, a method of identifying the industrial sources that exceed the emission rates established by the control is also given. Both methods are based on using a dispersion model, its adjoint model, and adjoint estimates of mean concentration of pollutant in monitored zones. The highlight of the new control is a new goal function that is minimized. Currently, it contains special weights for each industrial source in order to reduce the intensity of emissions of those sources that pollute the most. Conditions that show the convergence of the emission rates, prescribed by the control, to the original emission rates of the industrial sources are given (Theorems 4 and 5). These results ensure that the new emission rates of industrial sources (established by the control) will be as close as possible to the original emission rates throughout the entire period of application of the control. This creates the minimum possible restrictions on the functioning of industrial enterprises.

The new control method is the optimal short-term regulation of emissions from industrial sources. In the case when a dispersion model predicts an excess of the maximum permissible concentration of a pollutant in monitored zones, the method determines new, optimal to some extent, emission rates for each industrial source. From this point on, each industrial source should continue its work with reduced emission rates prescribed by the control. This prevents a violation of the air quality standard in the monitored zones selected in the industrial region.

The model of dispersion of a quasi-passive pollutant in a limited area with open boundaries used here during adverse weather conditions is considered separately from the dynamic model of the atmosphere, i.e., the wind velocity is assumed to be known from a dynamic model or observations [15]. As a result, the process of dispersion of pollutant is governed by the advection-diffusion equation.

It should be stressed that the control of emission rates of industrial sources uses the adjoint estimates of mean concentrations of pollutant in the monitered zones. The adjoint estimates are important because they explicitly depend on the number, positions and emission rates of the sources, as well as on the initial distribution of pollutant in the region. The adjoint model solutions in these estimates serve as weighting functions that provide valuable information about the contribution of each industrial source and the initial data to the pollution of each monitored zone. These properties make the adjoint estimates very effective in developing control strategies, as well as in studying the sensitivity of the dispersion model solution to changes in the intensity of sources and the initial distribution of pollutant in the region.

The ability of the new control method is illustrated by an example when the domain contains six pollution sources and one monitored zone. The example shows the effectiveness of the new goal function. Note that a similar approach can also be used to develop methods for cleaning water zones polluted by oil (the problem of bioremediation), and to prevent excessive pollution of urban areas with automobile emissions.

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Appendix A Construction of the adjoint model

The operator A^* of the adjoint model is adjoint to the operator A of dispersion model (1)–(6). The adjoint operator A^* is defined by means of the Lagrange identity $(A\phi, g) = (\phi, A^*g)$

[2], which in our case has the form

$$\int_D (A\phi) g \mathrm{d}\boldsymbol{r} = \int_D \phi(A^* g)\mathrm{d}\boldsymbol{r}.$$

Therefore, the model adjoint to (1)–(6) in the space-time domain $D \times (0, T)$ is defined by equations (10) and (11). Note that the wind velocity $\boldsymbol{U}(\boldsymbol{r}, t)$ and coefficients $\mu(\boldsymbol{r}, t)$ and $\sigma(\boldsymbol{r}, t)$ in the adjoint model are the same as in the dispersion model (1)–(6), while forcing $p(\boldsymbol{r}, t)$ is still undefined.

In order to explain the choice of the boundary conditions (12) at the inflow and outflow parts of boundary S, let us compare equations (1) and (10) provided that $f(\boldsymbol{r}, t) \equiv 0$ and $p(\boldsymbol{r}, t) \equiv 0$. One can see that equation (10), after using the substitution $t' = T - t$, differs from equation (1) only in the sign of velocity $\boldsymbol{U}$, and therefore, the inflow and outflow parts S^- and S^+ of the dispersion problem and adjoint problem are swapped. This explains why the boundary conditions (6) of dispersion problem are transformed into conditions (12) in the adjoint problem.

The choice of initial condition for the adjoint problem at the moment $t = T$ is explained by the fact that this problem is well posed only if solved from $t = T$ to $t = 0$. It follows from the fact that the time derivatives in (1) and (10) have different signs, while the operators A and A^* are both positive definite [3]:

$$(A\phi, \phi) = \int_D [\mathrm{div}(\boldsymbol{U}\phi) + \sigma\phi - \mathrm{div}(\mu\nabla\phi)]\phi \mathrm{d}\boldsymbol{r} > 0,$$
$$(A^* g, g) = \int_D [-\mathrm{div}(\boldsymbol{U}g) + \sigma g - \mathrm{div}(\mu\nabla g)] g \mathrm{d}\boldsymbol{r} > 0.$$

Appendix B Non-optimal control strategy

We now show that equation (24) also suggests a non-optimal strategy to control the emission rates. Indeed, let us define new emission rates $\hat{Q}_i(t)$ as

$$\hat{Q}_i(t) = Q_i(t) - \beta_i g(\boldsymbol{r}_i, t),$$
$$\beta_i = \frac{c_i + (c_0 - J_0) f_i}{\int_0^T g^2(\boldsymbol{r}_i, t)\mathrm{d}t}, \quad i = 1, 2, \ldots, N.$$

Then, multiplying the first equation by $g(\boldsymbol{r}_i, t)$ and integrating the result over time in the interval $(0, T)$ we obtain

$$\int_0^T \hat{Q}_i(t) g(\boldsymbol{r}_i, t)\mathrm{d}t = \int_0^T Q_i(t) g(\boldsymbol{r}_i, t)\mathrm{d}t - \beta_i \int_0^T g^2(\boldsymbol{r}_i, t)\mathrm{d}t.$$

The substitution of the coefficients β_i into the last equation and summing the resulting equation over i from $i = 1$ to $i = N$ gives

$$\sum_{i=1}^N \int_0^T \hat{Q}_i(t) g(\boldsymbol{r}_i, t)\mathrm{d}t$$
$$= \sum_{i=1}^N \int_0^T Q_i(t) g(\boldsymbol{r}_i, t)\mathrm{d}t - \sum_{i=1}^N (c_i + (c_0 - J_0) f_i).$$

Since

$$\sum_{i=1}^N \int_0^T Q_i(t) g(\boldsymbol{r}_i, t)\mathrm{d}t = \sum_{i=1}^N c_i \text{ and } \sum_{i=1}^N f_i = 1,$$

we obtain

$$\sum_{i=1}^N \int_0^T \hat{Q}_i(t) g(\boldsymbol{r}_i, t)\mathrm{d}t = -(c_0 - J_0)\sum_{i=1}^N f_i = J_0 - c_0.$$

Finally,

$$J(\phi_{\hat{Q}}) = c_0 + \sum_{i=1}^N \int_0^T \hat{Q}_i(t) g(\boldsymbol{r}_i, t)\mathrm{d}t = J_0.$$

Consequently, the emission rates $\hat{Q}_i(t)$ can also be considered as a non-optimal control of the mean concentration of pollutant in the zone Ω, provided that $\hat{Q}_i(t) \geqslant 0$ for all i.

Appendix C Proof of Theorem 4

The new emission rates $\hat{Q}_i(t)$ are defined as follows:

$$\begin{aligned}\hat{Q}_i(t) &= Q_i(t) - \beta_i g(\boldsymbol{r}_i, t)\\ &= Q_i(t) - (c_i + (c_0 - J_0) f_i)\frac{g(\boldsymbol{r}_i, t)}{\|g(\boldsymbol{r}_i, t)\|^2}.\end{aligned}$$

Since $f_i = \dfrac{c_i}{\sum_{j=1}^N c_j}$ then

$$\hat{Q}_i(t) = Q_i(t) - \frac{\sum_{j=1}^N c_j + (c_0 - J_0)}{\sum_{j=1}^N c_j} \frac{c_i}{\|g(\boldsymbol{r}_i, t)\|} \frac{g(\boldsymbol{r}_i, t)}{\|g(\boldsymbol{r}_i, t)\|}$$

and

$$\hat{Q}_i(t) = Q_i(t) - \frac{J(\phi_{\vec{Q}}) - J_0}{J(\phi_{\vec{Q}}) - c_0} \frac{c_i}{\|g(\boldsymbol{r}_i, t)\|} \frac{g(\boldsymbol{r}_i, t)}{\|g(\boldsymbol{r}_i, t)\|}.$$

On the other hand, the use of Schwarz's inequality leads to

$$\frac{c_i}{\|g(\boldsymbol{r}_i, t)\|} = \int_0^T Q_i(t)\frac{g(\boldsymbol{r}_i, t)}{\|g(\boldsymbol{r}_i, t)\|}\mathrm{d}t \leqslant \|Q_i\|.$$

Therefore,

$$\hat{Q}_i(t) \geqslant Q_i(t) - \frac{J(\phi_{\vec{Q}}) - J_0}{J(\phi_{\vec{Q}}) - c_0} \frac{g(\boldsymbol{r}_i, t)}{\|g(\boldsymbol{r}_i, t)\|} \|Q_i\|.$$

It follows from the last inequality that $\hat{Q}_i(t) \geqslant 0$ if and only if the condition (26) is satisfied.

To prove the uniform convergence of the emission rates, note that

$$\hat{Q}_i(t) = Q_i(t) - \frac{J(\phi_{\vec{Q}}) - J_0}{J(\phi_{\vec{Q}}) - c_0} \frac{c_i}{\|g(\boldsymbol{r}_i, t)\|} \frac{g(\boldsymbol{r}_i, t)}{\|g(\boldsymbol{r}_i, t)\|}$$

$$= Q_i(t) - (J(\phi_{\vec{Q}}) - J_0)\frac{c_i}{\sum\limits_{j=1}^{N} c_j}\frac{g(\boldsymbol{r}_i, t)}{\|g(\boldsymbol{r}_i, t)\|^2}.$$

The estimation $\frac{c_i}{\sum\limits_{j=1}^{N} c_j} < 1$ yields to

$$|\hat{Q}_i(t) - Q_i(t)| \leqslant (J(\phi_{\vec{Q}}) - J_0)\frac{g(\boldsymbol{r}_i, t)}{\|g(\boldsymbol{r}_i, t)\|^2}.$$

Defining M as the upper bound of $\frac{g(\boldsymbol{r}_i, t)}{\|g(\boldsymbol{r}_i, t)\|^2}$ for all i and $t \in (0, T)$, we obtain

$$|\hat{Q}_i(t) - Q_i(t)| \leqslant M(J(\phi_{\vec{Q}}) - J_0) \ \text{ for all } \ i \ \text{ and } \ t \in (0, T).$$

Thus, $\hat{Q}_i(t) \to Q_i$ uniformly on $(0, T)$ as $J(\phi_{\vec{Q}}) \to J_0$.

Appendix D Proof of Theorem 5

Note that

$$F(\hat{Q}) = \frac{1}{2}\sum_{j=1}^{N}\gamma_j^2\|Q_j - \hat{Q}_j(t)\|^2 = \frac{1}{2}\sum_{j=1}^{N}\gamma_j^2\beta_j^2\|g(\boldsymbol{r}_j, t)\|^2$$
$$= \frac{1}{2}\sum_{j=1}^{N}\gamma_j^2\frac{(c_j + (c_0 - J_0)f_j)^2}{\|g(\boldsymbol{r}_j, t)\|^2}.$$

Using that $f_j = \frac{c_j}{\sum\limits_{k=1}^{N} c_k}$ and $\gamma_j = \frac{1}{f_j}$ the last equation is simplified as

$$F(\hat{Q}) = \frac{1}{2}(J(\phi_{\vec{Q}}) - J_0)^2\sum_{j=1}^{N}\frac{1}{\|g(\boldsymbol{r}_j, t)\|^2}.$$

Due to (26) $\hat{Q} = (\hat{Q}_1, \dots, \hat{Q}_N) \in \Theta$, and therefore, $F_{\min} = F(\vec{Q}^*) \leqslant F(\hat{Q})$. Finally, for all i we obtain that

$$\frac{1}{2}\gamma_i^2\|Q_i - Q_i^*\|^2$$
$$\leqslant F(\vec{Q}^*) \leqslant F(\hat{Q}) = \frac{1}{2}(J(\phi_{\vec{Q}}) - J_0)^2\sum_{j=1}^{N}\frac{1}{\|g(\boldsymbol{r}_j, t)\|^2},$$

and then

$$\|Q_i - Q_i^*\|^2 \leqslant \Big(\frac{J(\phi_{\vec{Q}}) - J_0}{\gamma_i}\Big)^2\sum_{j=1}^{N}\frac{1}{\|g(\boldsymbol{r}_j, t)\|^2} \ \text{ for all } \ i.$$

Taking the limit on both sides of this estimation as $\gamma_i \to \infty$, or when $J(\phi_{\vec{Q}}) \to J_0$, we obtain that $\|Q_i - Q_i^*\| \to 0$.

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