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On a method of detecting the industrial plants which violate prescribed emission rates

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Abstract

A limited area pollution transport model and its adjoint are considered for controlling industrial emission rates and air quality. A method of detecting the industries, which ignore and violate the emission rates prescribed by an air quality control, is suggested. Some regularization techniques are considered to obtain the linear system with a well-conditioned matrix.

Keywords: Advection–diffusion-reaction equation; Control of industrial emissions

1. Introduction

The release of toxic gases from industrial plants constitutes a serious hazard to human health and environment. Therefore, it is of great importance to exercise control over industrial emissions. Besides, this problem is also of considerable mathematical interest (Penenko and Raputa, 1983). For example, let an air quality forecast (or a measurement) gives $J(\phi) > J_0$ in a zone Ω, where $J(\phi)$ is the mean concentration of a pollutant in Ω during some time interval and J_0 is a sanitary norm. Then one of the control strategies should be applied to improve air quality in the zone (Chiquetto and Mackett, 1995; Richards et al., 2002). Normally, any control strategy requires reducing the emission rates of industries so that to guarantee the fulfillment of the sanitary norm in the zone Ω: $J(\phi) \leq J_0$ (Parra-Guevara and Skiba, 2000a,b, 2002).

It is of practical importance to consider the situation when, in spite of applying an appropriate control, the measurements show unsatisfactory result again: $J(\phi) > J_0$, and hence, some industrial plants violate prescribed emission rates and are responsible for excessive polluting the zone Ω. This raises the question of detecting and sanctioning the plants-culprits. In the present work, a method of detecting such guilty plants is suggested. The method is readily applied to a three-dimensional pollution transport model (Brandt et al., 2001; Drago et al., 2001; Liu and Carroll, 1996; Skiba, 1993, 1997; Stokozov and Buesseler, 1999). However, for the simplicity of presentation, it is given here for a simple two-dimensional pollution transport model that can be obtained by integrat-

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ing the three-dimensional model over the inversion layer height (Skiba and Parra-Guevara, 2000).

Let D be a two-dimensional limited area containing N industrial plants. Denote by $r_i = (x_i, y_i)$ and $Q_i(t)$ the position and emission rate of the ith plant, respectively ($i = 1, 2,\ldots, N$). In a limited domain D and time interval $[0, T]$, we consider a typical advection–diffusion-reaction equation

$$\frac{\partial}{\partial t}\phi + \boldsymbol{U}\cdot\nabla\phi + \sigma\phi - \nabla\cdot\mu\,\nabla\phi = \sum_{i=1}^{N} Q_i(t)\,\delta(r - r_i) \quad (1)$$

where $\phi(r, t)$ is the concentration of a pollutant at a point $r = (x, y)$ and moment t, $\delta(r - r_i)$ is the Dirac function of the ith plant position, $\mu(r, t) > 0$ is the turbulent diffusion coefficient, and ∇ is the gradient. The parameter $\sigma(r, t) > 0$ characterizes the decay of $\phi(r, t)$ because of various physical and chemical processes. The wind velocity vector $\boldsymbol{U}(r, t) = \{u(r, t), v(r, t)\}$ is assumed to be known in D (from observed data or forecast model results) and to satisfy the continuity equation

$$\nabla\cdot\boldsymbol{U} = 0 \quad (2)$$

Eq. (1) is solved with the initial condition

$$\phi(r, 0) = \phi^0(r) \quad \text{at } t = 0 \quad (3)$$

and boundary conditions

$$\mu\frac{\partial}{\partial n}\phi - U_n\phi = 0 \quad \text{at } S^- \quad (4)$$

$$\mu\frac{\partial}{\partial n}\phi + 0 = S^+ \quad (5)$$

where $\phi^0(r)$ is a known initial distribution of the pollutant concentration in the domain D, and $U_n = \boldsymbol{U}\cdot\boldsymbol{n}$ is the projection of the wind velocity $\boldsymbol{U}$ on the unit outward normal $\boldsymbol{n}$ to the boundary S of the domain D (Fig. 1).

Since the pollution flux through the open boundary S of the limited area D is unknown, the boundary errors will propagate inside the domain by advection and diffusion, and perturb or destroy the exact solution. In addition, errors in the initial condition (3) and emission rates $Q_i(t)$ can also distort the solution. Thus it is important

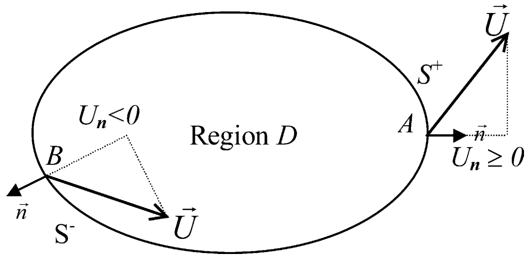

Fig. 1. A limited area D of the pollution transport problem, and the inflow part (S^-) and outflow part (S^+) of the boundary S of the domain D.

to select boundary conditions that are correct both physically and mathematically. To this end, we divide the boundary S of the domain D into the 'inflow' part S^- (where $U_n < 0$) and 'outflow' part S^+ (where $U_n \geq 0$) (Fig. 1). It is shown in Skiba and Parra-Guevara (2000) that problem (1)–(5) is well posed according to Hadamard (1923), i.e. it possesses unique solution, which continuously depends not only on the initial distribution $\phi^0(r)$, but also on the number N, emission rates $Q_i(t)$ and positions r_i of the industries. Numerical experiments with Eq. (1) show that parameterisation $\sigma\phi$ is quite good in the case of such contaminants as CO, SO_2, Pb, C, etc. (Shir and Shich, 1974).

Let us consider in the same space–time domain $D\times[0, T]$ one more (auxiliary mathematical) problem, which is adjoint to problems (1)–(5) in the sense of the Lagrange identity (Lyusternik and Sobolev, 1964; Marchuk and Skiba, 1976; Marchuk, 1986):

$$-\frac{\partial}{\partial t}g - \boldsymbol{U}\cdot\nabla g + \sigma g - \nabla\cdot\mu\nabla g = P(r, t) \quad (6)$$

$$\mu\frac{\partial}{\partial n}g = 0 \quad \text{at } S^- \quad (7)$$

$$\mu\frac{\partial}{\partial n}g + U_n g = 0 \quad \text{at } S^+ \quad (8)$$

$$g(r, T) = 0 \quad \text{at } t = T \quad (9)$$

The adjoint problem (6)–(9) uses the same functions $\boldsymbol{U}(r, t)$, $\mu(r, t)$ and $\sigma(r, t)$ as problem (1)–(5) and is also well posed (Skiba and Parra-Guevara, 2000) if solved backward in time (from $t = T$ to $t = 0$).

Let Ω be a zone (for example, an ecologically sensitive zone) in the domain D, and let

$$J(\phi) = \frac{1}{\tau|\Omega|} \int_{T-\tau}^{T} \int_{\Omega} \phi(r, t) \mathrm{d}r \, \mathrm{d}t \tag{10}$$

be the mean pollution concentration in the zone Ω and time interval $(T-\tau, T)$ of length τ. Obviously Eq. (10) can be obtained with the solution $\phi(r, t)$ to problem (1)–(5). Then adjoint problem (6)–(9) can be used to derive the so-called 'adjoint' estimate

$$J(\phi) = \sum_{i=1}^{N} \int_{0}^{T} g(r_i, t) Q_i(t) \mathrm{d}t + \int_{D} g(r, 0) \phi^0(r) \mathrm{d}r \tag{11}$$

which is equivalent to the 'direct' estimate (10) (Marchuk and Skiba, 1976). Here $|\Omega|$ is the area of Ω, and $g(r, t)$ is the solution to the adjoint problem (6)–(9) with the forcing (Skiba, 1993).

$$P(r, t) = \begin{cases} \dfrac{1}{\tau|\Omega|}, & \text{if } (r, t) \in \Omega \times (T-\tau, T) \\ 0, & \text{otherwise} \end{cases} \tag{12}$$

The principal significance of the adjoint estimate (11) is that it explicitly relates mean pollution concentration $J(\phi)$ in Ω with industrial emission rates $Q_i(t)$ and initial pollution distribution $\phi^0(r)$ through the values of $g(r, t)$ at the positions r_i of the pollution sources. Thus, non-negative solution $g(r, t)$ of the adjoint problem serves in Eq. (11) as a weight function. The peculiarities of the direct and adjoint estimates are discussed in detail in Skiba (1996, 1997). Unlike the solution $\phi(r, t)$ to problem (1)–(5), the solution $g(r, t)$ is independent of such parameters as the number N, positions r_i, and emission rates $Q_i(t)$ of the industries. This fact makes the adjoint estimate (11) very convenient both for studying the sensitivity of $\phi(r, t)$ with respect to variations in each of these parameters (Marchuk, 1986; Skiba, 1996, 1997, 1999) and for developing different strategies of the pollution control (Penenko and Raputa, 1983; Parra-Guevara and Skiba, 2000a,b, 2002). Indeed, no solution of problem (1)–(5) is required for using the basic sensitivity formula

$$\delta J(\phi) = \sum_{i=1}^{N} \int_{0}^{T} g(r_i, t) \delta Q_i(t) \mathrm{d}t + \int_{D} g(r, 0) \delta\phi^0(r) \mathrm{d}r \tag{13}$$

which is immediately obtained from Eq. (11) due to the linearity of the problem (Skiba, 1997). Moreover, the adjoint solution $g(r, t)$, once calculated, then can repeatedly be used to evaluate the contribution of variations in the emission rates $\delta Q_i(t)$ and initial distribution $\delta\phi^0(r)$ to variation $\delta J(\phi)$ of the pollutant concentration in the zone Ω. Eq. (13) also allows estimating the role of the number of the industries N and their positions r_i in polluting this zone. Unconditionally stable second-order finite difference schemes and numerical algorithms developed for the solution of problems (1)–(5) and (6)–(9) are described in detail in Skiba (1997, 1999).

2. Detection of the industries violating prescribed emission rates

Let J_0 be a sanitary norm and let a forecast model (or a measurement) gives unsatisfactory air quality result in the zone Ω: $J(\phi) > J_0$. Suppose that a control applied requires the industries to reduce their emission rates $Q_i(t)$ to such values $\tilde{Q}_i(t)$ that guarantee the fulfillment of the sanitary norm in Ω: $J(\phi) \leq J_0$. We now consider the situation when some industries ignored this requirement and continued to work with emission rates exceeding the prescribed values $\tilde{Q}_i(t)$. In other words, in spite of the control application, the measurements show again that $J(\phi) > J_0$, and hence, some plants are responsible for excessive polluting the zone Ω. This raises the question of detecting and sanctioning such plants. Though the detection problem is not trivial for time-dependent emission rates $Q_i(t)$, we now show that it can easily be solved for invariable emission rates. Note that the last requirement is not a strong restriction if the time interval $(0, T)$ is small enough.

Assume that within the interval $(0, T)$, the ith industry would work with a constant emission rate

Q_i if no control is applied, had to work with a constant rate $\tilde{Q}_i$ prescribed by a control, but has worked with an unknown constant rate $\bar{Q}_i$, and hence, $\delta Q_i = Q_i - \bar{Q}_i$ $(i = 1, 2,\ldots, N)$. Let $J(\phi)$ and $\bar{J}(\phi)$ be the mean pollutant concentrations in the zone Ω forecasted by the model before the control and measured after the control, respectively. Thus,

$$\delta J(\phi) = J(\phi) - \bar{J}(\phi) \tag{14}$$

is a known value. Let us choose K zones in the domain D $(K \geq N)$, and denote as $\delta J_k(\phi)$ the known value (Eq. (14)) obtained for the kth zone Ω_k $(k = 1, 2,\ldots, K)$. Assuming that at least one of the pollution estimates $J_k(\phi)$ exceeds a sanitary norm J_0, let us detect the industries, which are responsible for excessive polluting the zone(s). Denote the solution of adjoint problems (6)–(9) for the zone Ω_k by $g_k(r, t)$, and its value at the position r_i of the ith industry by $g_k(r_i, t)$ $(i = 1,\ldots, N)$. Fig. 2 shows isolines of the adjoint problem solution $g_k(r, t)$ calculated for a zone Ω_k at two moments: $t = T-60$ min and $t = T-90$ min ($T = 360$ min; $\tau = 60$ min), while a typical temporal behavior of functions $g_k(r_i, t)$ in interval $(0, T)$ is shown in Fig. 3 (see Skiba and Davydova-Belitskaya (2001); Davydova-Belitskaya et al. (2001) for more details). Taking into account that in our case, $\delta\phi^0(r) \equiv 0$, and δQ_i is constant for each i, the adjoint estimates (13) for K zones lead to a linear

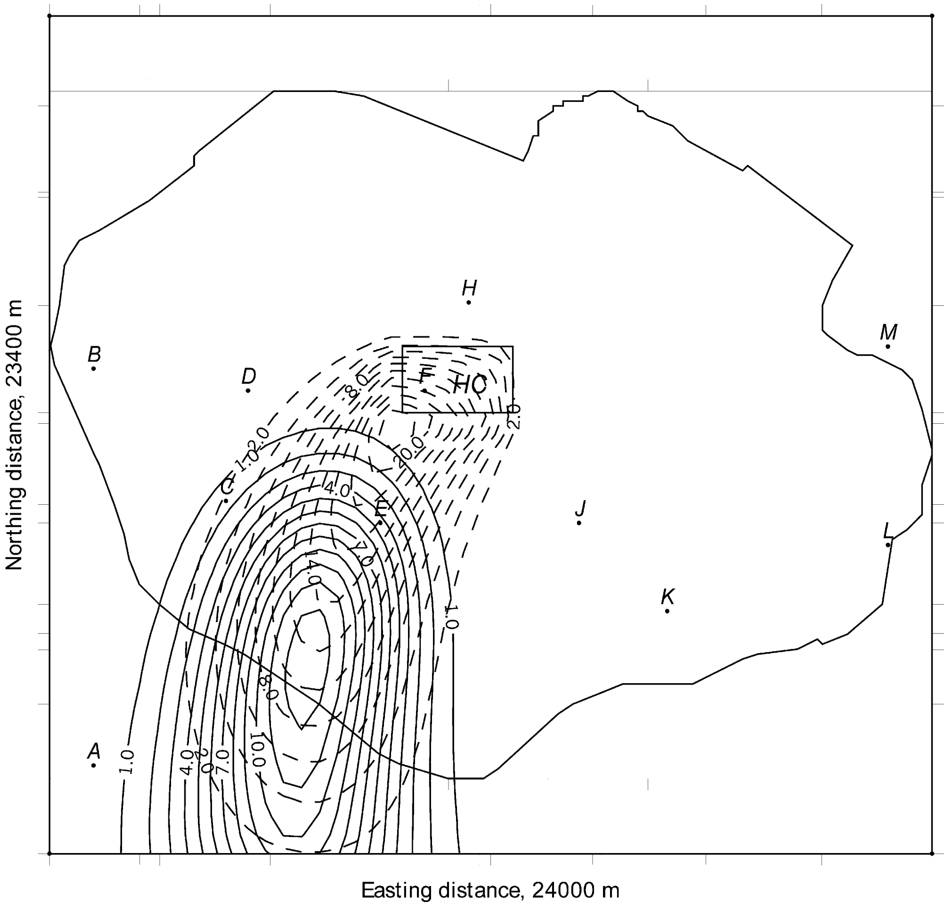

Fig. 2. Isolines of the adjoint solution $g_k(r, t)$ calculated for a zone Ω_k at two moments: $t = T-60$ min (dotted lines) and $t = T-90$ min (solid lines); $T = 360$ min.

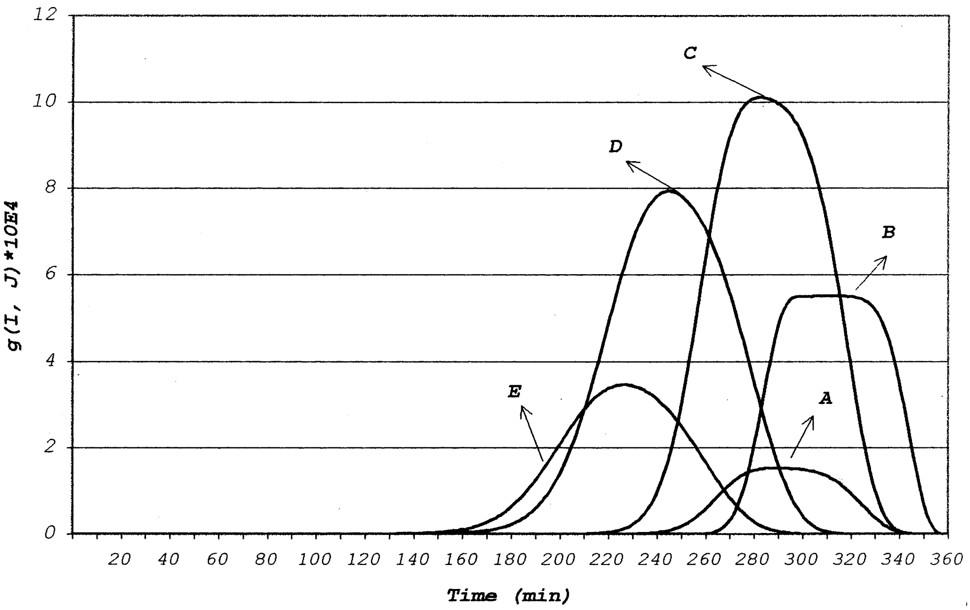

Fig. 3. A typical temporal behavior of the weight functions $g_k(r_i, t)$ in the interval $(0, T)$ for different industrial plants. The index k corresponds to the zone Ω_k, while r_i indicates the position of the ith industrial plant. The plants are denoted by the letters A, B, C, etc.

system

$$A\vec{x} = \vec{b} \tag{15}$$

or

$$\sum_{i=1}^{N} a_{ki}\delta Q_i = b_k \quad (k = 1, 2, ..., K) \tag{16}$$

with non-negative elements

$$a_{ik} = \int_0^T g_k(r_i, t)\mathrm{d}t \tag{17}$$

of the $N \times K$ matrix A $(i = 1,..., N;\ k = 1,..., K)$, and

$$b_k = \delta J_k(\phi) \tag{18}$$

The solution to Eq. (15) gives the values δQ_i, and hence, the values $\bar{Q}_i = Q_i - \delta Q_i$. Thus, if for some i, $\bar{Q}_i > \tilde{Q}_i$ then the ith plant has violated the prescribed emission rate.

We now make a few points.

(1) In (13) written for the zone Ω_k, the functions $g_k(r_i, t)$ in the integrals

$$\int_0^T g_k(r_i, t)\delta Q_i(t)\mathrm{d}t$$

are non-negative continuous functions. Therefore, according to the mean value theorem, we have

$$\int_0^T g_k(r_i, t)\delta Q_i(t)\mathrm{d}t = \delta Q_i^* \int_0^T g_k(r_i, t)\mathrm{d}t \tag{19}$$

where δQ_i^* is the mean value of $\delta Q_i(t)$ in time interval $(0, T)$, and hence, the same method in Eqs. (15)–(18) can also be applied for time depending emission rates with the aim to control the mean emission rates within interval $(0, T)$.

(2) If $K = N$ then the matrix A of the system in Eq. (15) is square. In this case it is important to estimate its condition number $\nu(A) = \|A\|\|A^{-1}\|$ (Stewart and Sun, 1990). In special simple cases when $\|B\| = \|E - A\| < 1$ in some norm (E is the identity matrix), the condition number can be evaluated as (Skiba, 2001).

$$\nu(A) = \|A\|\ \|A^{-1}\| \leq \frac{1 + \|E\|}{1 - \|B\|} \tag{20}$$

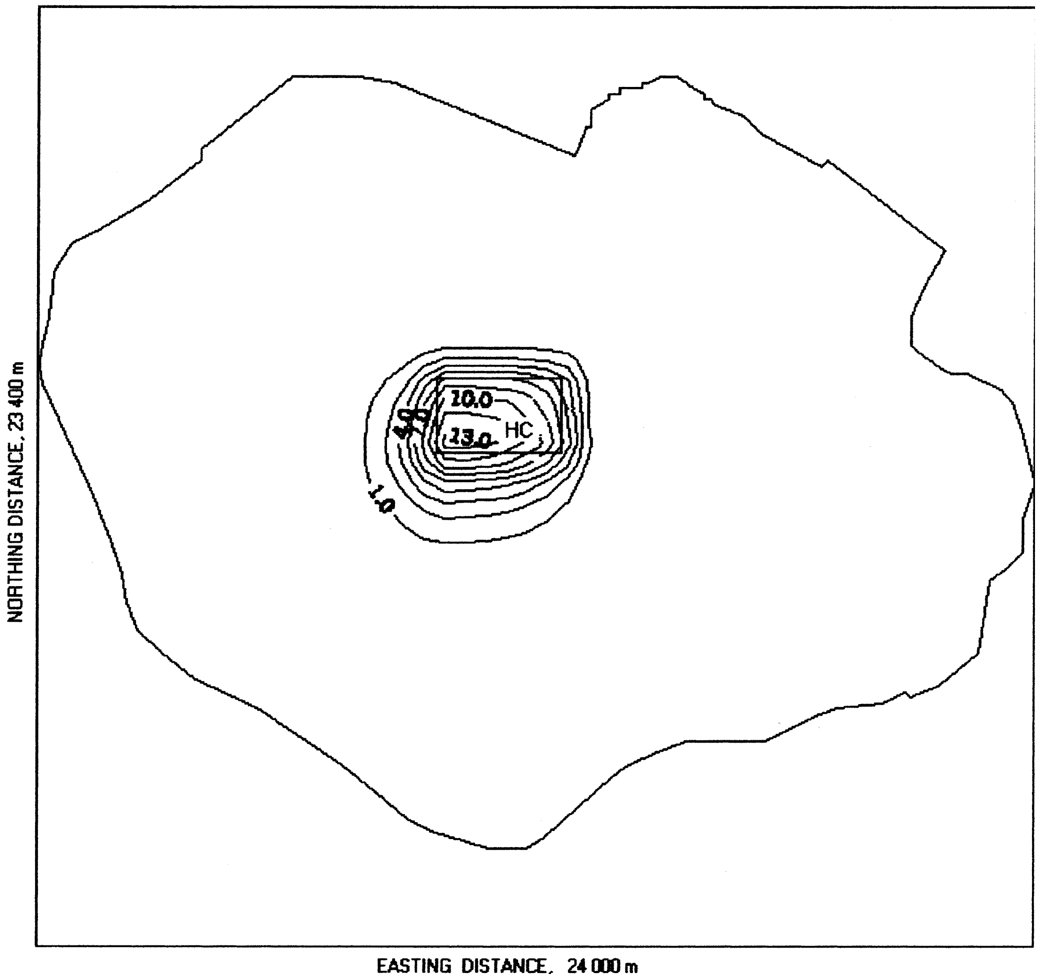

Fig. 4. Isolines of the adjoint solution $g_k(r, t)$ calculated for a zone Ω_k (Historical Center in Guadalajara City) at a moment t close to $T = 360$ min, while forcing (12) of the adjoint Eq. (6) is non-zero ($T = 360$ min; $\tau = 60$ min). The non-zero isolines are concentrated nearby the zone Ω_k.

Note, however, that in many cases, inequality $\|B\|<1$ is not satisfied. If the system in Eq. (15) is ill-conditioned (i.e. $\nu(A)$ is too large) then one of the regularization methods should be applied in order to resolve the system in Eq. (15) with a good accuracy (Bakhvalov, 1973).

(3) One of the regularization methods leading to a well-conditioned square matrix A consists in choosing the zones Ω_k in such a way that they do not intersect each other, besides, each of them contains just one industrial plant. If, in addition, we consider the problem in a small interval $(0, T)$ and take $\tau = T$ in Eq. (12), then isolines of the weight functions $g_k(r, t)$ calculated for a zone Ω_k will be concentrated just near the zone Ω_k (Fig. 4), and A will be a diagonally dominant matrix when $|a_{ii}| > \Sigma_{j \neq i} |a_{ij}|$ for each i ($i = 1, \ldots, N$).

(4) Sometimes, it is preferable to choose $K > N$. Then A is rectangular, and the system in Eq. (15) can be solved by means of least squares (Lawson and Hanson, 1974; Jacob, 1995):

$$\vec{x} = (A^T A)^{-1} A^T \vec{b} \tag{21}$$

The solution (21) is less sensitive with respect to errors in the system parameters and measurement.

(5) Sometimes, instead of the mean pollution concentrations $J_k(\phi)$ in the zones Ω_k, it is simpler to get mean values

$$J_k(\phi) = \frac{1}{\tau}\int_{T-\tau}^{T} \phi(c_k, t)\mathrm{d}t$$

of $\phi(r, t)$ in K points c_k of the domain D ($k = 1, \ldots, K$). In this case, each function $g_k(r, t)$ appearing in Eq. (17) is the solution to the adjoint problem (6)–(9) with the forcing

$$P_k(r, t) = \begin{cases} \frac{1}{\tau} & \text{if } r = c_k \quad \text{and } t \in (T - \tau, T) \\ 0 & \text{otherwise} \end{cases}$$

In the limit when the area of zone Ω_i is reduced just to the point r_i (the plant position), the pollution estimate $J_i(\phi)$ is transformed into the end-of-pipe control.

(6) The role of the initial distribution $\phi^0(r)$ in the air quality control decreases as interval $(0, T - \tau)$ grows (Skiba, 1993). Indeed, by Eq. (12), $P(r, t) \equiv 0$ within $(0, T - \tau)$, and in the absence of the forcing, the adjoint solution $g_k(r, 0)$, appearing in Eq. (11) as a weight function, decreases as $T - \tau$ grows due to the dissipation ($\sigma > 0$).

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References

Bakhvalov, N.S., 1973. Numerical Methods, vol. 1(in Russian). Nauka, Moscow.

Brandt, J., Christensen, J.H., Frohn, L.M., Zlatev, Z., 2001. Operational air pollution forecast modelling using the THOR system. Phys. Chem. Earth Part B Hydrol. Oceans Atmosphere 26, 117–122.

Chiquetto, S., Mackett, R., 1995. Modeling the effects of transport policies on air-pollution. Sci. Total Environ. 169, 265–271.

Davydova-Belitskaya, V., Skiba, Yu.N., Bulgakov, S.N., Martínez, A.Z., 2001. Modelación matemática de los niveles de contaminación en la ciudad de Guadalajara, Jalisco, Mexico. Parte II. Modelo numérico de transporte de contaminantes y su adjunto. Rev. Int. Contam. Ambiental 17, 97–107.

Drago, M., Cescon, B., Iovenitti, L., 2001. A three-dimensional numerical model for eutrophication and pollutant transport. Ecol. Model. 145, 17–34.

Hadamard, J., 1923. Lectures on Cauchy's Problem in Linear Partial Differential Equations. Dover, New York, p. 1923.

Jacob, B., 1995. Linear Functions and Matrix Theory. Springer-Verlag, New York.

Lawson, Ch.L., Hanson, R.J., 1974. Solving Least Squares Problem. Prentice-Hall, Englewood Cliffs, NJ.

Liu, M., Carroll, J.J., 1996. A high-resolution air pollution model suitable for dispersion studies in complex terrain. Monthly Weather Rev. 124, 2396–2409.

Lyusternik, L., Sobolev, V., 1964. Elements of Functional Analysis. Ungar, New York.

Marchuk, G.I., 1986. Mathematical Models in Environmental Problems. Elsevier, New York.

Marchuk, G.I., Skiba, Yu.N., 1976. Numerical calculation of the conjugate problem for a model of the thermal interaction of the atmosphere with the oceans and continents. Izvestiya Atmospheric Oceanic Phys. 12, 279–284.

Parra-Guevara, D., Skiba, Yu.N., 2000a. Optimización de emisiones industriales para la protección de zonas ecológicas. Atmósfera 13, 27–38.

Parra-Guevara, D., Skiba, Yu.N., 2000b. Industrial pollution transport. Part II: control of industrial emissions. Environ. Model. Assess. 5, 177–184.

Parra-Guevara, D., Skiba, Yu.N., 2002. Elements of the mathematical modelling in the control of pollutants emissions, Ecolog. Model., submitted for publication.

Penenko, V.V., Raputa, V.F., 1983. Some models for optimizing the operation of the atmospheric-pollution sources. Sov. Meteorol. Hydrol. 2, 46–54.

Richards, J.P., Glegg, G.A., Cullinane, S., Wallace, H.E., 2002. Policy, principle, and practice in industrial pollution control: views from the regulatory interface. Environ. Manag. 29, 182–194.

Shir, C.C., Shich, L.J., 1974. A generalized urban air pollution model and its application to the study of SO_2 distributions in the St. Louis metropolitan area. J. Appl. Meteorol. 13, 185–204.

Skiba, Yu.N., 1993. Balanced and absolutely stable implicit schemes for the main and adjoint pollutant transport equations in limited area. Rev. Int. Contam. Ambiental 9, 39–51.

Skiba, Yu.N., 1996. Dual oil concentration estimates in ecologically sensitive zones. Environ. Monit. Assess. 43, 139–151.

Skiba, Yu.N., 1997. Air pollution estimates. World Resource Rev. 9, 542–556.
Skiba, Yu.N., 1999. Direct and adjoint oil spill estimates. Environ. Monit. Assess. 59, 95–109.
Skiba, Yu.N., 2001. Introducción a los Métodos Numéricos. DGPFE, UNAM, México.
Skiba, Yu.N., Davydova-Belitskaya, V., 2001. Air pollution estimates in Guadalajara City. Environ. Model. Assess. 7, 153–162.
Skiba, Yu.N., Parra-Guevara, D., 2000. Industrial pollution transport. Part I: formulation of the problem and air pollution estimates. Environ. Model. Assess. 5, 169–175.
Stewart, G.W., Sun, J.-G., 1990. Matrix Perturbation Theory. Academic Press, New York.
Stokozov, N.A., Buesseler, K.O., 1999. Mixing model for the north-west Black Sea using Sr-90 and salinity as tracers. J. Environ. Radioactivity 43, 173–186.