IDENTIFICATION OF SOURCES OF ATMOSPHERIC POLLUTION

S.A. Soldatenko, S.S. Suvorov, O.M. Sobolevskii, and V.S. Komarov

A.F. Mozhaiskii Military Space Engineering Academy, St. Petersburg
Institute of Atmospheric Optics,
Siberian Branch of the Russian Academy of Sciences, Tomsk
Received January 16, 1995

A method is proposed for a solution of the inverse problem of determining the position, number, strength, and type of pollution sources based on the use of an equation adjoint of the semiempirical equation of turbulent diffusion. Stationary point pulsed and continual sources are considered. The results of qualitative analysis of a model of the spread of pollutant are presented.

A problem of identification of the parameters and number of sources of the atmospheric aerosol pollution from measurements of the pollutant concentration is of interest for solving many scientific and practical problems, in particular, when considering a problem of ecological monitoring. In a number of papers (see, for example, Refs. 1 and 2) the problem of determining the position and strength of a single continual source was studied. At the same time, a variety of the processes of polluting is not exhausted by this case only. A problem of pollution identification is considered in this paper in the lack of *a priori* information about position, type, number, and strength of sources, what is a typical situation when estimating the degree of anthropogenic impact onto the protected environment.

Let us introduce into consideration a certain spatiotemporal domain $\Omega\times\Omega_t$ and denote the distribution function of the pollutant concentration by $\varphi(\mathbf{x}, t)$ and the function describing sources by $f(\mathbf{x}, t)$, where $\mathbf{x} \in 2\Omega$ and $t \in \Omega_t$. We introduce the Cartesian coordinate system in Ω. Denoting an operator describing the spread of pollutant by L, we write down a basic model in the form

$$L_\varphi = f , \quad (1)$$

where

$$L = \frac{\partial}{\partial t} + \mathbf{u}\ \mathrm{grad} - \mathrm{div}\ \mu\ \mathrm{grad} - \frac{\partial}{\partial z}\ \nu\ \frac{\partial}{\partial z} . \quad (2)$$

Initial and boundary conditions are formulated as follows:

$$\varphi = 0 \text{ at } t = 0 , \quad \varphi = 0 \text{ on } \Psi \text{ for } \mathbf{u}_n < 0 ,$$

$$\frac{\partial\varphi}{\partial n} = 0 \text{ on } \Psi \text{ for } \mathbf{u}_n \geq 0 ,$$

$$\frac{\partial\varphi}{\partial z} = \alpha\ \varphi + M \text{ on } \Psi_0 ,$$

$$\frac{\partial\varphi}{\partial z} = 0 \text{ on } \Psi_H , \ w = 0 \text{ at } z = 0 \text{ and } z = H ,$$

where $\mathbf{u} = (u, v, w)$ and u, v, and w are the velocity components along the x, y, and z axes, respectively; Ψ, Ψ_0, and Ψ_{H} are the boundaries of Ω; α is the coefficient of entrainment of the pollutant with a surface; μ and ν are the horizontal and vertical diffusion coefficients; and, M is the surface source of the pollutant.

Processes of sedimentation and self–induced ascent are taken into account in the vertical component of wind velocity w (as in Ref. 3). For definiteness, we assume that the pollutant is monodisperse and inert. Now we consider practically significant cases of a stationary point or pulsed source of pollutant in Ω. We use δ–function for the formal description of a single point source.[4] Then we have for the pulsed source

$$f(\mathbf{x}, t) = Q\ \delta(\mathbf{x} - \mathbf{x}_\xi)\ \delta(t - t_\xi) , \quad (3)$$

and for the continuous one

$$f(\mathbf{x}, t) = Q(t)\ \delta(\mathbf{x} - \mathbf{x}_\xi) . \quad (4)$$

In Eqs. (3) and (4) Q is the strength of emission, $\mathbf{x}_\xi$ is the source coordinate, and t_ξ is the source lifetime. Let the continuous source strength be constant in time, i.e., Q = const.

Now we investigate the salient features of the pollutant field evolution in Ω for different source types corresponding to the right–hand side of Eq. (1) in the form of Eq. (3) or (4). It should be noted that Eq. (1) describes a system with distributed parameters, i.e., its phase pattern has an infinite dimensionality. The phase patterns shown in Fig. 1 were obtained following the approach outlined in Ref. 5. For continuous source (Fig. 1 *a*), heterocline trajectory is observed, and the corresponding solution has the form of a travelling wave of front type. For a single pulsed source (Fig. 1 *b*), homocline trajectory and solution of a pulse type were obtained. The presence of several continual sources does not change the system behavior qualitatively. However, it should be noted that for several pulsed sources, periodic trajectory originating from the homocline loop is observed (Fig. 1 *c*). So, taking into account that the singular points A and B correspond to the stationary solution of Eq. (1), it may be concluded that:

– analysis of the dynamics of change in $\partial\varphi/\partial t$ can provide a basis for determination of the source type;

– it is desirable to identify continuous sources after termination of a transient period, i.e., after setting up of a stationary regime;

– uncertainty in the number of pulsed sources, unlike continuous ones, can be eliminated by an analysis of the field φ on the number of maxima (the point c).

0235-6880/95/07 515-04 \$02.00

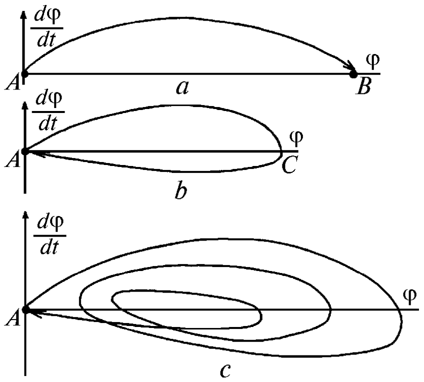

FIG. 1. Trajectories for equation (1) for single continuous source (a), single pulsed source (b), and several pulsed sources (c) of pollutant.

To solve the inverse problem, we use the adjoint model

$$L^* \varphi^* = f^* \tag{5}$$

with the initial and boundary conditions:

$$\varphi^* = 0 \text{ at } t = T \ , \ \varphi^* = 0 \text{ on } \Psi \text{ for } \mathbf{u}_n < 0 \ ,$$

$$\mu \frac{\partial \varphi^*}{\partial n} + \mathbf{u}_n \varphi^* = 0 \text{ on } \Psi \text{ for } \mathbf{u}_n \geq 0 \ ,$$

$$\frac{\partial \varphi^*}{\partial z} = \alpha \varphi + M \text{ on } \Psi_0 \ ,$$

$$\frac{\partial \varphi^*}{\partial z} = 0 \text{ on } \Psi_H \ , \quad w = 0 \text{ for } z = 0 \text{ and } z = H \ .$$

The operator L^* adjoint of the operator L of basic problem (1) can be obtained based on the Lagrange identity[6]:

$$(\varphi^*, L \varphi) = (\varphi^*, L^* \varphi^*) \tag{6}$$

and has the form

$$L^* = -\frac{\partial}{\partial t} + \mathbf{u} \text{ grad} - \text{div } \mu \text{ grad} - \frac{\partial}{\partial z} \nu \frac{\partial}{\partial z} \ . \tag{7}$$

Allowing for Eqs. (1) and (5), Eq. (6) can be reduced to the form

$$(\varphi^*, f) = (\varphi, f^*) \ . \tag{8}$$

Let us denote the Green's functions of the basic and adjoint operators by $G_\xi(\mathbf{x}, t)$ and $G_r^*(\mathbf{x}, t^*)$, respectively (subscripts ξ and r correspond to the source coordinates $\mathbf{x}_\xi$ and the position of a point of concentration measurements $\mathbf{x}_r$). By definition, the functions $G_\xi(\mathbf{x}, t)$ and $G_r^*(\mathbf{x}, t^*)$ can be obtained by solving Eqs. (2) and (5) with the right–hand side in the form of Eq. (3) or (4) for the source of unit strength (for G_r^* , $\mathbf{x}_\xi$ is substituted by $\mathbf{x}_r$). Then using Eq. (8) we obtain

$$(G_r^*(\mathbf{x}, t^*), \delta(\mathbf{x} - \mathbf{x}_\xi)) = (G_\xi(\mathbf{x}, t), \delta(\mathbf{x} - \mathbf{x}_r)) \ .$$

Hence,

$$G_r^*(\mathbf{x}_\xi, t^*) = G_\xi(\mathbf{x}_r, t) \tag{9}$$

at $t^* = t$. Reciprocity of the Green's functions of the basic and adjoint operators provides a basis for solving the problem of identification. The requirement $t^* = t$ is not too burdensome when determining the continuous source parameters if the system is in the stationary regime (the point B in Fig. 1 *a*); however, it essentially complicates the solution of the problem in the case of pulsed sources.

Now, using $G_\xi(\mathbf{x}, t)$ we represent the solution of basic model (1) at the point $\mathbf{x} \in \Omega$ for each point source described by Eq. (3) or (4) with the coordinates $\mathbf{x}_\xi$ and strength Q_ξ as follows:

$$\varphi(\mathbf{x}, t) = Q_\xi \, G_\xi(\mathbf{x}, t) \ . \tag{10}$$

Having written the solution of Eq. (1) in the form of Eq. (10) for the point of source $\mathbf{x}_\xi$ and having arbitrarily chosen a point with coordinate $\mathbf{x}_r$, after some transformations we obtain

$$\varphi(\mathbf{x}_\xi, t) \ / \ [G_\xi(\mathbf{x}_r , t)] = Q_\xi \, R_\xi(\mathbf{x}_r , t) \ , \tag{11}$$

where $R_\xi = G_\xi(\mathbf{x}_\xi, t)/G_\xi(\mathbf{x}_r , t)$ characterizes a change in the solution sensitivity. So, to produce the concentration $\varphi(\mathbf{x}_\xi, t)$, the source strength must be increased by $R_\xi(\mathbf{x}_r , t)$ as this source moves to the point $\mathbf{x}_r$. Allowing for Eq. (9) and having generalized Eq. (11) on the whole domain Ω we introduce a function of the necessary strength S

$$S_r(\mathbf{x}, t) = \varphi(\mathbf{x}_r, t) \ / \ G_r^*(\mathbf{x}, t^*) \ , \tag{12}$$

which is defined as the source strength necessary for producing the concentration φ at the point $\mathbf{x}_r$ as a function of its coordinates $\mathbf{x}$. In other words, if $\varphi(\mathbf{x}_r , t)$ is known (measured) then $S_r(\mathbf{x}, t)$ is the strength of a fictitious source placed at the point $\mathbf{x}$, which produces this concentration.

Let us discuss a problem of existence of a solution to inverse problem using Eq. (12). For vivid presentation in one–dimensional case, we consider the following expression:

$$S_{r1}(\mathbf{x}_a) = S_{r2}(\mathbf{x}_b) \ , \tag{13}$$

where the correspondence to the measurement points with coordinates $\mathbf{x}_{r1}$ and $\mathbf{x}_{r2}$, $\mathbf{x}_a \in \Omega$, $\mathbf{x}_b \in \Omega$ is indicated by the subscripts $r1$ and $r2$, and the symbol t is omitted on the assumption that the stationary regime is considered. With allowance made for Eqs. (12) and (10), expression (13) has the form

$$G_\xi(\mathbf{x}_{r1}) \ / \ G^*_{r1}(\mathbf{x}_a) = G_\xi(\mathbf{x}_{r1}) \ / \ G^*_{r2}(\mathbf{x}_b) \ . \tag{14}$$

It follows from Eq. (9) that at least one point exists with the coordinate $\mathbf{x}_a = \mathbf{x}_b = \mathbf{x}_\xi$ where Eq. (14) is valid.

Now proceeding from the qualitative difference between mechanisms of the pollutant field formation with continuous and pulsed sources, algorithms for solving the inverse problem for different source types are considered separately. In the case of a single continuous source, the solution is reduced to finding the point $\mathbf{x}$ ($\mathbf{x} = \mathbf{x}_\xi$) for which

$$S_{r1}(\mathbf{x}) = S_{r2}(\mathbf{x}) = \ldots = S_{rn}(\mathbf{x}) \ , \tag{15}$$

where n is the necessary number of points of measuring the pollutant concentration corresponding to the number of the sought–after parameters. In particular, for the plane case with measurement points on the plume axis (i.e., the problem is one–dimensional), finding the point satisfying Eq. (15) can be reduced to minimization of functional of the following form:

$$\arg\min\, (S_r(\mathbf{x}) - S_{r1}(\mathbf{x}))^2\ ,\quad \mathbf{x} \in \Omega\ .$$

A form of necessary functional depends on dimensionality of the problem being solved. After determination of the source coordinate x_ξ, the source strength is obtained from relation (12).

In the presence of p continuous sources the determination of their parameters in general is reduced to a solution of the system of equations

$$GQ = F\ . \tag{16}$$

Elements of the matrix G are $g_{ij} = G^*_{ri}(x_{\xi j})$, $Q = [Q_1, \ldots, Q_p]^{\mathrm{T}}$, $F = [\varphi_{r1}, \ldots, \varphi_{rn}]^{\mathrm{T}}$, $i = 1(1)n$, $j = 1(1)\,p$, $x_{\xi j}$ are the coordinates of the jth source, and φ_{rj} are the measurement in the ith point. Let us denote a contribution of the jth source by φ^j, then after some transformations Eq. (16) can be reduced to the following form:

$$G'\,Q' = \varphi_{r1}\ , \tag{17}$$

where the elements of the matrices G' and Q' are represented as

$$g'_{i\,j} = \left(\frac{S_{r1}(\mathbf{x}_{\xi j})}{S_{ri}(\mathbf{x}_{\xi j})} - \frac{S_{r1}(\mathbf{x}_{\xi p})}{S_{ri}(\mathbf{x}_{\xi p})}\right),$$

$$g'_{i\,j} = \varphi^j_{r1}\left(1 - \frac{S_{r1}(\mathbf{x}_{\xi p})}{S_{ri}(\mathbf{x}_{\xi p})}\right)^{-1},\quad i = 2(1)\ n\ ,\ j = 1(1)\ p - 1\ .$$

After solving Eq. (17) for $x_{\xi j}$ and φ^j_{r1}, the source strengths are derived from Eq. (12) by substitution of φ by φ^j_{r1}. The value of φ^j_{r1} is determined from the principle of solution superposition. A certain complication of the elements of the matrices Q and G is compensated by reduction of their dimensionality and feasibility to identify the source making a maximum contribution to the concentration value.

In the case of identification of pulsed sources, a problem arises connected with uncertain time of emission (accordingly, time of integration of the adjoint problem). By analogy with the case of continual sources, the function of necessary strength of the pulsed source S' is introduced. We assume that the pollutant emission of strength Q occured at the moment t_ξ at the point x_ξ. Starting from a certain moment T_{r0} ($T_{r0} = t_\xi + \tau$, $\tau \geq 0$), the coordinates $\mathbf{x}^m_{rk}$ and maximum values of field φ (the point C in Fig. 1 *b*) denoted by φ^m_{rk} ($\varphi^m_{rk} = \varphi(\mathbf{x}^m_{rk})$) are determined at regular time intervals Δ_t at the moments T_{rk} ($k = 0(1)\ l$, $T_{rk} = T_{r0} + k\Delta_t = t_\xi + \tau + k\Delta_t$). Then

$$S'(t^*) = \varphi^{\,m}_{rk}\ /\ G^{*m}_{rk}(t^*)\ ,\qquad t^* \in [T_{rk},\ 0]\ , \tag{18}$$

where $G^{*m}_{rk}(t^*)$ is the maximum fundamental solution of Eq. (5). Now we consider the identification of a single pulsed source. For every moment T_{rk}, the function (18) is constructed, then determination of the time of emission t_ξ is reduced to finding the moments t^*_{rk} for which

$$S'_{r0}(t^*_{r0}) = S'_{r1}(t^*_{r1}) = \ldots = S'_{rl}(t^*_{rl}) \tag{19}$$

with $t_\xi = T_{rk} - t^*_{rk}$. The source coordinates $\mathbf{x}_\xi$ provide the maximum of the function G^*_{rk} upon integrating problem (5) over the time $T_{rk} - t^*_{rk}$, and the strength Q can be obtained from Eq. (18). The identification of p ($p > 1$) pulsed sources in general is reduced to solving the system of equations (16) for a certain moment T_{rk} with the corresponding matrix elements of the form

$$g_{ij} = G_{\xi j}(\mathbf{x}^{mi},\ T_{rk})\ ,\quad Q = [Q_1,\ \ldots,\ Q_p]^{\mathrm{T}}\ ,$$

$$F = [\varphi^{\,m1}_{rk},\ \ldots,\ \varphi^{\,mp}_{rk}]^{\mathrm{T}}\ ,\quad i = 1(1)\ p\ ,\quad j = 1(1)\ p\ .$$

We assume that the measurement intervals Δ_t are regular as before and denote the interval between the instant of emission from the jth source and the start of measurements of the field φ by τ_j : $\tau_j = T_{rk} - t_{\xi j}$. Similarly to the case of a single pulsed source, the position $\mathbf{x}^{mj}_{rk}$ and value φ^{mj}_{rk} of each maximum of the field φ at the moment T_{rk} ($\varphi^{mj}_{rk} = \varphi(\mathbf{x}^{mj}_{rk},\ T_{rk})$) are determined. Then the following expression is valid for each ith maximum:

$$\varphi^{\,mi}_{rk} = Q_i G^{\,*mi}_{rk}(\tau_i + k\,\Delta_t) = \sum_{j=1}^{p} Q_j G^{\,*i}_{rk}(\mathbf{x}_{\xi j},\ \tau_i + k\Delta_t)\ ,\ j \neq i\ . \tag{20}$$

In the right–hand side of Eq. (20), the first term determines contribution to the ith maximum of the field φ from the ith source, the second term determines contribution from the other $p - 1$ sources, j denotes the current numbers of all sources except i, and G^{*i}_{rk} is the solution of problem (5) with the right–hand side in the form $f = \delta(\mathbf{x} - x^{mi}_{rk})\ \delta(t - T_{rk})$. If the second term in the right–hand side of Eq. (20) is small and can be ignored, the identification of p pulsed sources is reduced to the application of a procedure of determining the single source parameters corresponding to each of p maxima of the field φ. This situation arises for sources separated in time or (and) space and is characterized qualitatively by the phase pattern shown in Fig. 1 *b* (i.e., the mapping point returns to the equilibrium state A). Otherwise the system behavior is characterized by Fig. 1 *c*, i.e., by existence of a limit cycle. Then the identification of p pulsed sources is reduced to solving the system of equations

$$GQ = F^m\ , \tag{21}$$

where the elements of the matrix G have the form

$$g_{kj} = G^{\,*j}_{rk}(\mathbf{x}_{\xi j},\ \tau_j + k\ \Delta_t)\ \text{for}\ j \neq 1\ ,$$

$$g_{k1} = G^{\,*mj}_{rk}(\tau_j + k\ \Delta_t)\ ,\quad Q = [Q_1,\ \ldots,\ Q_p]^{\mathrm{T}}\ ,$$

$$F^m = [\varphi^{\,m1}_{r1},\ \ldots,\ \varphi^{\,m1}_{rn}]^{\mathrm{T}}\ ,\ k = 0(1)\ l\ ,\ j = 1(1)\ p\ .$$

Since the number of sources is *a priori* unknown, a problem of choosing the needed algorithm arises. To solve this problem at a certain point $\mathbf{x}_r$, the derivative $\partial\varphi/\partial t$ is analyzed and the source type is identified at the first step.

Two cases are possible: the presence of continuous sources (Fig. 1 *a*) and of pulsed sources (Fig. 1 *b* or *c*). In the first case, the hypothesis on the presence of a single source is set up and the source parameters are determined from Eqs. (15) and (12) using the measurements of the concentration in two different groups of points. The obtained solutions are compared. The identification is considered as completed when these solutions fall within the uncertainty interval. Otherwise the hypothesis on the presence of the several sources is accepted. The number of sought–after sources is increased by unity and the system of equations (17) is solved for measurements in two groups of points. The number of sought–after sources is increased until the solutions fall within the uncertainty interval γ. For example, from the results of numerical experiments it was found that the expression for the uncertainty interval of the source strength has the form

$$\gamma_Q = \chi\, \varphi + 0.44\, \xi\, v + 0.69\, \xi\, \mu ,$$

where χ_s is the relative error in assignment of the element s. When detecting pulsed sources, the uncertainty in their number is eliminated by an analysis of the field φ on the number of maxima p. When $p > 1$, it is necessary to estimate the second term in the right–hand side of Eq. (20) based on possibly available *a priori* information or analysis of $\partial\varphi/\partial t$, and to use the approach based on Eq. (19) (a single source or separated sources) or to solve the system of equations (21).

Realization of the identification procedure is reduced to splitting of the operator of conjugated model (5) with processes and coordinates[7] and difference approximation of the obtained operators. We note that in the problems of the pollutant source identification a special attention must be given to numerical realization of the advection step that is caused by the presence of discontinuity of the function φ due to influence of point sources of pollutant.

Based on a series of numerical experiments using widespread schemes for solving similar problems (e.g., those of McCormak, Laks–Wendroff, FCT, and TVD) it may be concluded that the explicit TVD scheme provides the best approximation (from the considered schemes) of the exact solution over all interval including discontinuity points. To match the digitization intervals in time and space, inexplicit scheme, for example, Krank–Nikolson scheme, should be used. Equations (15), (17), (19), and (21) are solved with the use of standard procedures.[8,9]

The results of numerical experiments showed that the approximation error in splitting of operators (2) and (6) is smaller than 1%. For statistical estimation of quality of determining position and strength of sources, a series of numerical experiments was carried out using settlement Siverskii of the Leningrad region as an example. For a sample of 10 000 measurements of the pollutant concentration it was obtained that, for example, for a single continuous source with the strength $Q = 5$ g/s the confidence limits ($P = 0.95$) are 660 m, 270 m, and 0.6 g/s for x, y, and Q, respectively.

REFERENCES

1. A.I. Krylova and V.F. Raputa, Meteorol. Gidrol., No. 5, 29–35 (1993).
2. V.V. Penenko, V.F. Raputa, and A.V. Panarin, Meteorol. Gidrol., No. 11, 15–23 (1985).
3. S.A. Soldatenko and O.M. Sobolevskii, Atmos. Oceanic Opt. **7**, No. 2, 112–116 (1994).
4. M.E. Berlyand, *Current Problems of Atmospheric Diffusion and Pollution of the Atmosphere* (Gidrometeoizdat, Leningrad, 1995), 250 pp.
5. M. Holodniok, A. Klich, et al., *Methods of Analysis of Nonlinear Dynamic Models* (Mir, Moscow, 1991), 365 pp.
6. G.I. Marchuk, *Mathematical Simulation in Environmental Problems* (Nauka, Moscow, 1982), 319 pp.
7. G.I. Marchuk, *Splitting Methods* (Nauka, Moscow, 1988), 263 pp.
8. A.A. Amosov, Dubinskii, et al., *Numerical Methods for Engineers* (Vyssh. Shkola, Moscow, 1994), 544 pp.
9. N.S. Bakhvalov, *Numerical Methods* (Nauka, Moscow, 1975), Vol. 1, 631 pp.