Inverse problem of determination of the atmospheric pollution source parameters based on data on the underlying surface deposit density

O.V. Botalova, A.I. Borodulin, S.R. Sarmanaev, and S.S. Kotlyarova

Institute of Aerobiology, State Research Center of Virology and Biotechnology "Vector," Kol'tsovo, Novosibirsk Region

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In the mathematical modeling of propagation of atmospheric contaminants the inverse problems are understood as problems of determining the type, coordinates, and power of the pollution source based on the data on the contaminant concentration given in the limited amount of observation points. The paper describes the problem of determining the coordinates and the power of a stationary source of atmospheric pollutants based on the use of the equation conjugated with a semiempirical equation of turbulent diffusion. When solving the inverse problem, the values of the particle deposit density accumulated in a snow cover during the winter period are used as the input data.

There are two classes of problems describing the propagation of aerosol and gaseous atmospheric pollutants. The first class is associated to direct problems, that is, the pollution concentration must be found based on the known characteristics of its sources. The second class represents the inverse problems when it is required to determine the type, coordinates, and the power of the pollution sources from information about the pollution concentration measured in a series of control points. At the Euler approach to description of the turbulent diffusion, the use of a semiempirical equation of turbulent diffusion is the most successful. For stationary conditions of pollution propagation considered below, it has the form[1]

$$\frac{\partial \overline{U}_i\,\overline{C}}{\partial x_i} - \frac{\partial}{\partial x_i} K_{ij} \frac{\partial \overline{C}}{\partial x_j} = \overline{Q} \quad (i, j = \overline{1,3}), \tag{1}$$

where $\overline{C}$ and $\overline{U}_i$ are the mathematical expectations of the pollution concentration and components of wind velocity; K_{ij} are the components of tensor of coefficients of turbulent diffusion (it is assumed that $K_{ij} = K_i$ at $i = j$ and $K_{ij} = 0$ at $i \neq j$); $\overline{Q}$ is the term describing the pollution source; $x = x_1$ and $y = x_2$ correspond to horizontal coordinates, and $z = x_3$ corresponds to vertical coordinates. The bar denotes averaging over a statistical ensemble. The repeated indices mean a summation. The solution of direct problem is set in the rectangular region G with the surface S consisting of the side surface Σ, the lower basis Σ_0 (at $z = 0$) and the upper basis Σ_H (at $z = H$). The system of boundary conditions for Eq. (1) is:

$$\overline{C} = 0 \text{ at } \Sigma,\ \Sigma_H;\quad K_z \frac{\partial \overline{C}}{\partial z} + V_s\,\overline{C} = \beta \overline{C} \text{ at } \Sigma_0, \tag{2}$$

where V_s is the rate of particle sedimentation; β is the parameter of the impurity interaction with the underlying surface.

The Institute of Aerobiology of SRC VB "Vector" together with the Institute of Atmospheric Optics SB RAS, ICKC SB RAS, and ICMMG SB RAS systematically study the biogenic component of the atmospheric aerosol in the south of Western Siberia.[6–9] One of the problems, solved within the framework of this project, is the mathematical simulation of propagation of atmospheric bioaerosols, search and identification of their local and global sources.[9] Climatic conditions of Siberia are characterized by the stable snow cover observed over a long period of time, which is an accumulator of the atmospheric precipitation. The goal of this work is to solve the problem of determining the parameters of sources of atmospheric impurities based on data on the precipitation density on the underlying surface.

Determine the power of a point stationary source of atmospheric impurities located at a point with the coordinates x_0, y_0, z_0. Let

$$\overline{Q} = Q_0\,\delta(x - x_0)\,\delta(y - y_0)\,\delta(z - z_0), \tag{3}$$

where Q_0 is the power of the impurity source. Owing to the presence of snow cover practically in the entire region of interest, one can consider approximately that β = const over the entire area. The quantity Q_0 and the source coordinate can be found, for example, by repeated solving of the direct problem (1) and (2). However, this approach is very cumbersome. Therefore, those methods of solving inverse problems are of particular practical interest, which are based on the use of the turbulent diffusion equation.[2] For example, the problem of determination of the source coordinates and power requires the use of such type of equations. In this case we use as input data the values of the particle precipitation density, accumulated in the snow cover during the winter period.

The mathematical expectation of the precipitation density of aerosol deposition $\overline{D} = \overline{D}(x, y)$ is[1]

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$$\overline{D} = \int_0^T \left(V_s \overline{C} + K_z \frac{\partial \overline{C}}{\partial z} \right) \Bigg|_{z=0} \mathrm{d}t = \beta T \overline{C} \Big|_{z=0}, \qquad (4)$$

where T is the time of accumulation of aerosol particles in the snow cover.

According to the Marchuk method,[2] for the formulation of a conjugate problem, Eq. (1) is multiplied by a certain function C_* and integrated over the region G. As the result, we have the expression

$$\int_G \overline{C} \left(-\frac{\partial \overline{U}_i C_*}{\partial x_i} - \frac{\partial}{\partial x_i} K_{ij} \frac{\partial C_*}{\partial x_j} \right) \mathrm{d}G + \int_S \overline{U}_i \overline{C} C_* \, \mathrm{d}S +$$

$$+ \int_S \left(C_* K_{ij} \frac{\partial \overline{C}}{\partial x_j} - \overline{C} K_{ij} \frac{\partial C_*}{\partial x_j} \right) \mathrm{d}S = \int_G C_* \overline{Q} \, \mathrm{d}G. \qquad (5)$$

It is assumed that in Eq. (5)

$$\frac{\partial \overline{U}_i C_*}{\partial x_i} + \frac{\partial}{\partial x_i} K_{ij} \frac{\partial C_*}{\partial x_j} = 0. \qquad (6)$$

Now separate out at the underlying surface Σ_0 two regions: the region of sampling Σ_1, and the region Σ_{0-1} supplementing Σ_1 up to Σ_0. The following system of boundary conditions for Eq. (6)

$$C_* = 0 \text{ at } \Sigma, \Sigma_H; \; \beta C_* - K_z \frac{\partial C_*}{\partial z} = \varphi_0 \text{ at } \Sigma_1;$$

$$\beta C_* - K_z \frac{\partial C_*}{\partial z} = 0 \text{ at } \Sigma_{0-1}, \qquad (7)$$

where φ_0 is the arbitrary constant, transforms Eq. (5) into the identity

$$\int_{\Sigma_1} \frac{\overline{D} \varphi_0}{\beta T} \mathrm{d}x \mathrm{d}y = \int_G C_* \overline{Q} \, \mathrm{d}G. \qquad (8)$$

In contrast to the classical formulation of the Marchuk method, intended for solution of inverse problems, the obtained integral identity (8) uses the values of the integral impurity concentration measured not at some point inside the region G but at boundary points of the region under consideration.

Equation (8) makes it possible to solve the inverse problem of determination of the source's type, coordinates, and power from the values of the density of the atmospheric impurity deposit measured in a series of reference points. A similar problem for the integral impurity concentration, measured at points above the underlying surface, was considered by us in Refs. 3–9. In Ref. 3, we formulated the problem of minimization of functional of the observational data and the results of solving the conjugate equations. Such an approach, for example, enables one to solve the problem of finding the characteristics of a point source of atmospheric impurities based on a limited array of observed values of their concentration. These methods were also generalized to solve the problem of finding the characteristics of ensemble of the point sources.[5]

Further calculation and reasoning will be made orienting to solution of the above-mentioned problem with the use of the finite-difference methods. Assume that the point impurity source is located at the mth node $(m = \overline{1, M})$ of difference grid covering the region G and having coordinates x_m, y_m, z_m. Now we consider several small areas S_k $(k = \overline{1, K})$, at which snow samples were taken. In view of relations (8), (3), and (4) we have

$$\overline{D}_k \varphi_0 S_k / (\beta T) = Q_{km} \overline{C}_{*k} (x_m, y_m, z_m), \qquad (9)$$

where $\overline{C}_{*k}$ is the solution of the conjugate problem (6), (7) for a small area Σ_k with the area S_k; D_k is the measured value of the deposit density on the kth area. The values of Q_{km} represent the power of a stationary source located in mth node of the calculation template and creating the measured value of the deposit density $\overline{D}_k$ at the small area Σ_k. Thus, after k-multiple solution of conjugate problems (6) and (7), Eq. (9) determines a set of values Q_{km} in each of M nodes of the calculation template. Now we determine the quantities:

$$\overline{Q}_m = \frac{1}{K} \sum_{k=1}^{K} Q_{km}; \quad \sigma_m^2 = \frac{1}{K-1} \sum_{k=1}^{K} \left(Q_{km} - \overline{Q}_m \right)^2. \qquad (10)$$

By the condition of uniqueness of the inverse problem solution, only in one node of the calculation template a source can be found, which determines the values of the impurity deposit density measured at the given small areas Σ_k. It is evident that the node of the calculating template with the minimal value of dispersion σ_m^2 estimates the unknown coordinates of the source, and the value $\overline{Q}_m$ estimates the unknown source power Q_0.

Now we consider the results of the numerical experiment demonstrating the applicability of the above approach. A stationary impurity source was located in the left-bank region of Novosibirsk at a point with the coordinates: $x_0 = 3.5$ km; $y_0 = 8$ km; $z_0 = 50$ m (see Fig. 1).

The particle diameter was set equal to 2 μm, and the source power $Q_0 = 1000$ arbitrary units. The city buildings are gray in the figure. The river Ob, dividing the city into two parts, is dark gray. In the calculations, the meteorological conditions were typical for winter conditions at western wind of 3 m/s velocity at the level $z = 2$ m above the underlying surface. The wind velocity field over the city was determined by the numerical-analytical model.[11]

At the first stage the direct problem (1) and (2) was solved, i.e., the concentration fields of impurity and the deposit density accumulated on the underlying surface were calculated. Five black isolines show the deposit density of aerosol particles.

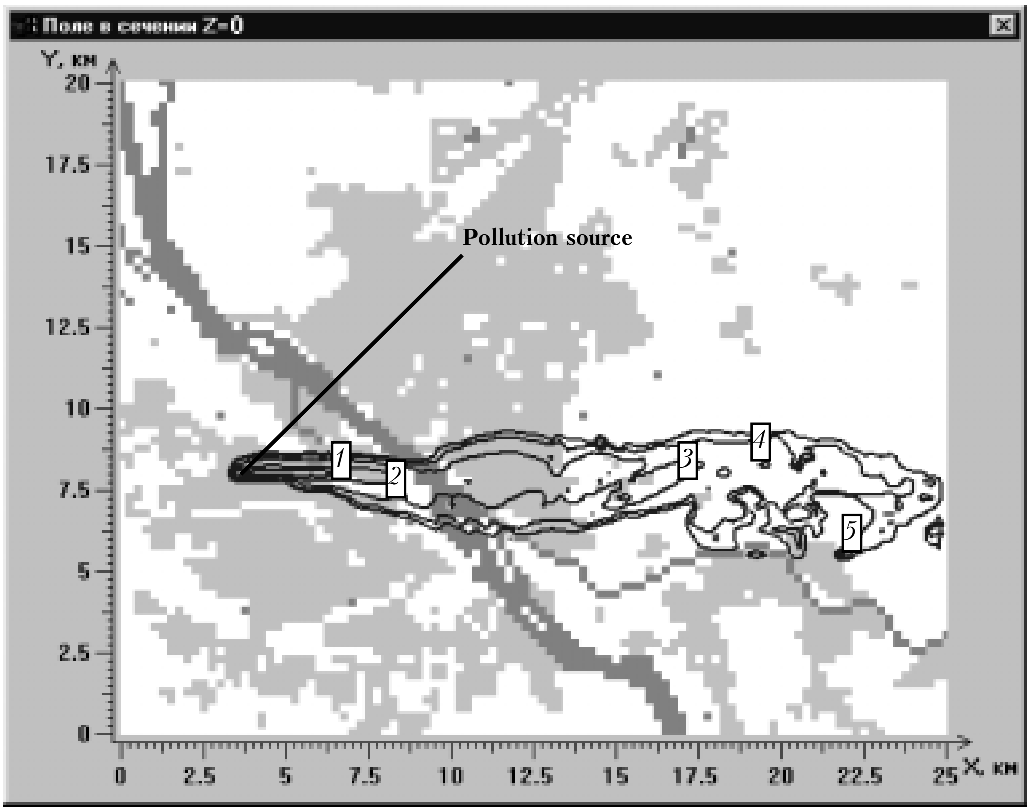

Fig. 1. Isolines of the deposit density of atmospheric impurities on the underlying surface.

Their values are 0.8, 0.5, 0.2, 0.09, and 0.06 arbitrary units. The inner isoline has a maximal value of the deposit density, and the others are shown in order of their decreasing values. To solve the inverse problem, five reference points were selected numbered in the figure from 1 to 5. The values of the deposit density at these points and their coordinates, calculated by solving the direct problem, are given in Table 1.

Table 1. Parameters of reference points chosen for calculations

Point number	Coordinates of reference points, km		Calculated values of the deposit density, arbitrary units
	x	y	
1	7	8.5	0.091
2	8	8	0.551
3	17	8	0.223
4	19	8.5	0.106
5	22.5	6	0.095

Then the conjugate problem (6) and (7) has been solved. By relationships (9) and (10) in every node of the calculation template the values of Q_{km} were found, the values of $\overline{Q}_m$ were calculated, and the nodes of the calculation template were chosen corresponding to the minimum of dispersion σ_m^2. The calculation results are given in Table 2.

The obtained data show that the reconstruction of parameters of the aerosol impurity source, according to the values of the particle deposit density accumulated in the snow cover, can be realized with a high degree of accuracy at three and more reference points. It is seen that the use of only two reference points introduces significant errors in calculations. These data are marked gray in Table 2. In future, when determining the characteristics of impurity sources based on the results of measurements,

Table 2. Results of determination of source characteristics

Point number	The calculated source power $\overline{Q}_m$, arb. units	Minimal value of dispersion σ_m^2, arb. units	Source coordinates, x, y (km), and z (m)
1, 2	998	0.015	3.5; 8.0; 50
1, 3	2880	0.087	1.0; 8.5; 205
1, 4	894	0.010	4.5; 8.3; 45
2, 3, 4	998	0.196	3.5; 8.0; 50
3, 4, 5	998	0.462	3.5; 8.0; 50
2, 4, 5	998	0.335	3.5; 8.0; 50
1, 2, 3, 4	998	0.180	3.5; 8.0; 50

one should take into account a spread of the experimentally obtained values of the deposit density. The influence of the measurement errors on the results of the inverse problem solution was analyzed by us in Ref. 12.

Thus, this paper considers the problem of determination of the atmospheric pollution source parameters from the data on the deposit density on the underlying surface. This approach can be used for analysis of experimental data on the biogenic component of the atmospheric aerosol, search and identification of their possible local sources based on the measured values of the deposit density of aerosol particles accumulated by the underlying surface during winter period. Therefore, the snow sampling in spring and analysis of the samples for the content of living microorganisms and particles of protein nature represent a unique possibility to supplement and generalize the results of atmospheric observations.[10]

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