DETERMINATION OF SOME CHARACTERISTICS OF AN AEROSOL POLLUTION SOURCE BY SOLVING THE INVERSE PROBLEM OF POLLUTANT SPREAD IN THE ATMOSPHERE

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We propose here an economical and stable method to determine coordinates of an instant point-like source of aerosol pollution and an amount of emitted pollutants from values of integral pollutant concentration measured at several spatial points. The method is based on solution of a conjugate equation of turbulent diffusion. Two examples are considered. In the first one, a pollutant spreads over a homogeneous underlying surface. The second case is pollutant spreading over the city of Novosibirsk with its real terrain, housing system, green and water areas. Calculations over the area with homogeneous underlying surface give good results already for two reference points, at which the integral pollutant concentration is measured. When simulating the spread over the real terrain, estimates are less accurate, but still quite satisfactory for practical applications of the proposed method.

Suppose that monitoring stations have detected a sharp increase in concentration of a certain dangerous substance due to a concealed emission from one of numerous plants situated in a given region. What plant of the possible ones is guilty? What amount of the substance has been emitted? How large will be the area with the substance concentration exceeding the maximum permissible level? Determination of coordinates of the pollution source and the amount of the emitted pollutant from a limited measurement data (solution of an inverse problem) is a typical problem, which ecological services often face in their real practice. Urgency and practical importance of development of efficient methods and algorithms for solving problems of such a kind are evident.

There exist several approaches to solution of inverse problems. Usually, iteration methods (the method of steepest descent, the method of random walk, etc.),[1] in which every iteration step includes solution of a direct problem, are used. Naturally, such calculation methods are time-expensive. Attempts to obtain an analytical solution to the inverse problem face obstacles. Most often, they manifest themselves as ambiguity of a solution. "Having not guessed" an initial approximation, which is necessary to start the iteration process, one may not only lose some solutions, but also solve the problem incorrectly. Versatile methods for choosing the initial approximation have not been developed yet.

Another approach is based on solution of an equation, conjugate with the equation of turbulent diffusion. The problem of mathematical simulation of some processes associated with environmental protection on the basis of conjugate equations was first formulated by G.I. Marchuk in the early 70s. Then it was further developed in Refs. 2–5.

When solving inverse problems, the conjugate formulation, reflecting the principle of duality,[2] allows development of algorithms, which in some cases appear to be the best ones both in the analysis of inverse problems and in their solution. It is important that they eliminate the necessity to solve repeatedly direct and conjugate problems.

In this paper, we propose an economical and stable method to determine coordinates of an instant point-like pollution source and an amount of a substance emitted into the atmosphere from values of the integral pollutant concentration measured at several spatial points. The proposed method is based on solution of the conjugate equation of turbulent diffusion.

The integral concentration of an aerosol pollutant defined as

$$D = \int\limits_0^\infty C(t)\,\mathrm{d}t$$

in the domain Ω $(0 \le x \le X, \ 0 \le y \le Y, \ 0 \le z \le Z)$ satisfies the following equation:

$$U\,\frac{\partial D}{\partial x} + V\,\frac{\partial D}{\partial y} + (W - V_s)\,\frac{\partial D}{\partial z} =$$
$$= \frac{\partial}{\partial x}\,K_x\,\frac{\partial D}{\partial x} + \frac{\partial}{\partial y}\,K_y\,\frac{\partial D}{\partial y} + \frac{\partial}{\partial z}\,K_z\,\frac{\partial D}{\partial z} + R \qquad (1)$$

with the boundary conditions

$$D\,\Big|_{\substack{x=0,\,X \\ y=0,\,Y}} = D\,\big|_{z=Z} = 0;$$

$$\left(K_z\,\frac{\partial D}{\partial z} + V_s\,D - \beta D\right)\Big|_{z=0} = 0, \qquad (2)$$

where C is the mathematical expectation of the pollutant concentration; U, V, and W are the x-, y- and z-components of the mean wind velocity; K_x, K_y, and K_z are the corresponding coefficients of turbulent diffusion; V_s is the sedimentation rate of aerosol particles; β is the parameter describing the pollutant interaction with the underlying surface; $R(x, y, z)$ is the function describing the pollutant sources.

The stationary equation (1) for the instant point-like pollution source can be derived from the semi-empirical equation of turbulent diffusion[6] by time integration from zero to infinity. According to Ref. 2, we introduce the parameter D_* satisfying the equation

$$-U\frac{\partial D_*}{\partial x} - V\frac{\partial D_*}{\partial y} - (W - V_s)\frac{\partial D_*}{\partial z} =$$

$$= \frac{\partial}{\partial x}K_x\frac{\partial D_*}{\partial x} + \frac{\partial}{\partial y}K_y\frac{\partial D_*}{\partial y} + \frac{\partial}{\partial z}K_z\frac{\partial D_*}{\partial z} + R_* , \qquad (3)$$

conjugate to Eq. (1). Here $R_* = R_*(x, y, z)$ is the function explained below. The boundary conditions for the function D_* are set the following:

$$D_*\Big|_{\substack{x = 0, X \\ y = 0, Y}} = D_*\Big|_{z = Z} = 0;$$

$$\left(K_z\frac{\partial D_*}{\partial z} - \beta D_*\right)\Big|_{z = 0} = 0. \qquad (4)$$

Upon multiplication of Eq. (1) by D_* and Eq. (3) by D, subtract one from another and integrate the result over the domain Ω. Taking into account boundary conditions (2) and (4), we obtain the integral identity

$$\int_\Omega R_* D \, dV = \int_\Omega R D_* \, dV, \qquad (5)$$

where dV is the volume element of the domain Ω. Let

$$J = \int_\Omega R_* D \, dV \qquad (6)$$

be a linear functional depending on D. It can be calculated based on the solution of problem (1) and (2). It follows from Eq. (5) that the same functional can be calculated by solving conjugate problem (3) and (4). This property demonstrates the principle of duality as applied to representation of functionals of type (6).

The meaning of R_* and D_* can be explained by the following example. Let

$$R_* = Q_* \delta_3(x - x_k, y - y_k, z - z_k), \qquad (7)$$

where δ_3 is the 3D delta function[1]; x_k, y_k, z_k are the coordinates of a point in the domain Ω. Then

$$J = Q_* D(x_k, y_k, z_k) = Q_* D_k. \qquad (8)$$

It follows herefrom that the functional J governs the integral value of the pollutant concentration D_k at a given point accurate to the factor Q_*. On the other hand, upon setting R_* and solving system (3) and (4) for the function D_*, we can calculate the integral concentration D_k by making use of Eq. (5). Thus, D_* is Green's function, that is, the function describing the influence of sources given by the function $R(x, y, z)$ on the integral concentration D_k at a certain point.

Suppose that an instant emission of a pollutant of mass Q_m occurred at time t_0 at an unknown point x_m, y_m, z_m, that is, $R = Q_m\delta_3(x - x_m, y - y_m, z - z_m)$. Suppose also that the integral concentration D_k was detected at reference points with the coordinates x_k, y_k, z_k ($k = 1, 2, ..., K$). The function R_* is set by relation (7). For each of K reference points, we solve problem (3) and (4) and find the set of K Green's functions D_{*k}. Then, according to Eqs. (5) and (8), we obtain the equation for unknown values of Q_{km}. They correspond to the mass of the substance emitted by the source situated at the mth point of the difference grid and forming the integral concentration D_k at the kth point:

$$Q_{*k} D_k = \int_\Omega R D_* \, dV = Q_{km} D_{*km} ;$$

$$k = 1, ..., K; \ m = 1, ..., M,$$

where D_{*km} are values of the Green's function at the mth point of the difference grid for the source situated at the kth reference point; M is the number of difference grid nodes. Thus, in each node m the K values of the mass Q_{km} corresponding to the set of K measured values of integral concentration D_k are determined. Then the mean value $\overline{Q}_m$ and the variance σ_m^2 are calculated for the mth node:

$$\overline{Q}_m = \frac{1}{k}\sum_{k=1}^{K} Q_{km} ; \quad \sigma_m^2 = \frac{1}{k - 1}\sum_{k=1}^{K}(Q_{km} - \overline{Q}_m)^2. \qquad (9)$$

By virtue of the property of uniqueness of the solution to the problem of pollutant spread, the source, which forms the measured values of the integral concentration D_k at the points x_k, y_k, z_k, can be situated at only one grid point. It is evident that the point with minimum variance corresponds to sought coordinates of the source, and the corresponding value $\overline{Q}_m$ is the sought mass of the pollutant emitted. It can be shown that the source coordinates and mass can be determined if and only if $K \geq 2$.

Consider two examples. In the first case, pollutant spread occurs over a plain homogeneous surface. In the second one, the pollutant spreads over a real terrain with various types of surfaces (housing system with various house height, steppe, forest, water areas, etc.).

To obtain values of the integral concentration at the reference points, direct problem (1) and (2) was solved prior to solution of inverse problem (3) and (4). At the point x_0 = 12 km, y_0 = 20 km, z_0 = 50 m (z_0 is the vertical coordinate) (see Fig. 1) an instant emission of the pollutant with the total mass Q_0 took place at 03:00 p.m. of the local time. The pollutant was carried away by particles 10 μm in diameter. Calculations have been performed for the meteorological conditions, typical of Novosibirsk on June 25. The city was blown with the south-west wind with velocity of 3 m/s at the height of the wind vane at a suburban meteorological station. Wind velocity fields over the area and the integral pollutant concentration were calculated by the method described in Ref. 7.

Figure 1 exemplifies the results of calculations for the first case. Integral concentration isolines are drawn for z = 50 m. The inner isoline is drawn for the integral concentration equal to 3.7 relative units, the others are drawn for 1.8, 1.2, 0.46, 0.23, and 0.09 relative units, respectively. The integral concentration at the reference points 1, 2, ... , 6 is equal to 1.8, 1.1, 0.74, 0.56, 0.46, and 0.37 relative units, respectively.
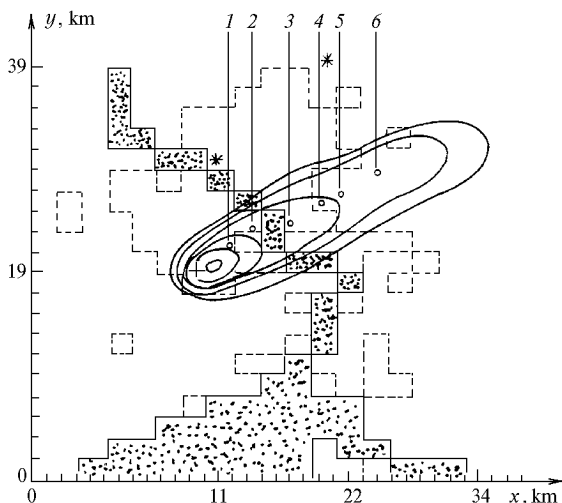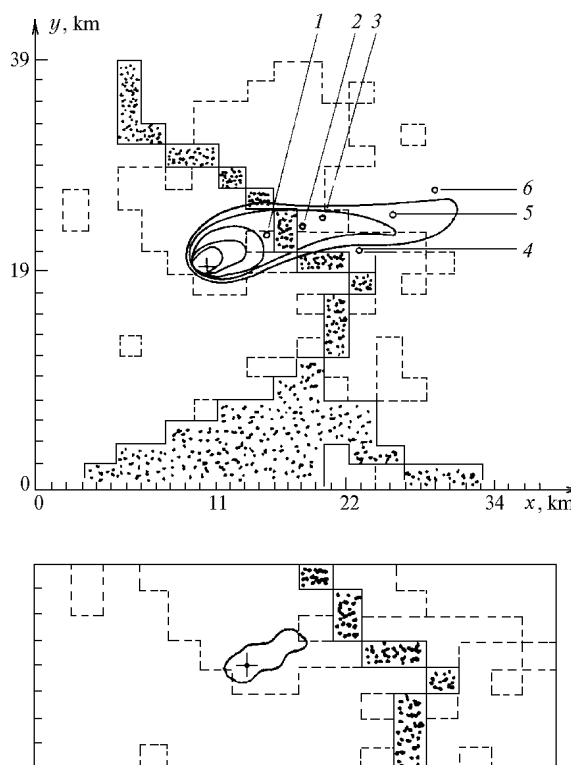

FIGx 1x An example of integral concentration isolines for the case of pollutant spread over a plane and homogeneous surfacex The numbered circles are the reference pointsx The source is marked by a crossx The dashed line is for boundary of Novosibirsk; the dotted area is the River Ob and the water reservoirx

Then we solved inverse problem (3) and (4) to determine the source coordinates and the amount of the emitted substance. When only two reference points (the first and the third ones) were used, the coordinates corresponding to the minimum variance σ_m^2 coincided with the initially set coordinates of the source. The reconstructed value of the mass differed from the initial value by less than 3%. The calculations revealed that the increase in the number of reference points, as well as changes in their arrangement, practically does not

influence the accuracy of determination of the source characteristics over a homogeneous and plane area.

The integral concentration field obtained for the second case is shown in the upper part of Fig. 2. The inner isoline is drawn for the integral concentration of 3.7 relative units, others are drawn for 1.8, 1.2, 0.46, and 0.23 relative units, respectively. In spite of relatively plain terrain in Novosibirsk, the integral concentration fields differ considerably from those calculated over a homogeneous underlying surface. The integral concentration at the reference points 1, 2, ... , 6 is equal to 1.2, 0.70, 0.47, 0.017, 0.39, and 0.13 relative units, respectively. For the second case, we failed to obtain results with the so high accuracy as in the first one.

FIGx 2x An example of integral concentration isolines for the case of pollutant spread over a real terrain (Novosibirsk)x The designations are the same as in Figx 1x The fragment in the lower part presents the isoline of variance σ_m^2 obtained for two reference pointsx

In most cases, the error in determination of the source coordinates is equal to one horizontal step (2 km) of the difference grid and two to three vertical steps (50 m). The mass of the emitted substance, corresponding to the minimum variance, can be determined accurate to 20% when using all the six reference points. If the number of the reference points is reduced to two, the errors increase up to 80%. However, the isoline of variance σ_m^2 presented in the lower part of Fig. 2 for the case of two reference points used localizes the source quite satisfactorily. If there are

more than three reference points, the accuracy of determination of the source coordinates is comparable with that achieved in calculations over a homogeneous surface. Calculations with different sets of initial data indicate the stability of the obtained results and efficiency of the algorithm.

Additional test calculations with analytically set components of wind velocity, at which the maximum value of the vertical velocity varied from 0.1 to 1.2 m/s, have shown that the accuracy of reconstruction of the source coordinates and the mass of the emitted substance is in this case approximately the same as in the first example (a homogeneous surface). This indicates that the observed increase in the error of reconstruction of the sought parameters in the second example is caused by insufficient accuracy in calculations of the wind velocity components, rather than the proposed method for solution of the inverse problem.

Finally, let us present some results of calculations with real data obtained by the Novosibirsk Air Pollution Monitoring Service. On 5th of May, 1994, the following values of the nitrogen dioxide concentration were detected at two stations marked by asterisks in Fig. 1: $C_1 = 0.89$ and $C_2 = 1.48$ mg/m^3, what several times exceeds the maximum permissible concentration equal to 0.085 mg/m^3. Other ten monitoring stations situated in different districts have recorded an order of magnitude less concentration values, which could be interpreted as background ones, although they are comparable with the maximum permissible concentration and typical of Novosibirsk. This is why this background concentration was neglected. Approximately the same concentration values were observed during 12 hours, while the wind direction and velocity remained almost constant. The assumed emission seems lasting for about 10-12 hours with almost constant power, rather than instant one. In this connection it should be noted that if Eq. (1) is interpreted as a stationary equation for the pollutant concentration, $\overline{Q}_m$ is an estimate of the source power.

The Table I presents the first five obtained minimum values of σ_m, the corresponding values of $\overline{Q}_m$, which are interpreted as the source power taking into account the above notes, and the coordinates x_m, y_m, and z_m of the assumed sources (the vertical step in these calculations was 2 m).

Several large industrial plants are situated in Novosibirsk near the points with the tabulated coordinates. Now, with an additional information about the type of emission, the height of smoke stacks, and peculiarities of technological processes, the plant can be determined, which most probably is guilty of the pollution.

TABLE Ix

σ_m, kg/s	$\overline{Q}_m$, kg/s	x_m, km	y_m, km	z_m, km
1.0	340	10	22	506
5.0	130	6	24	206
5.3	180	4	22	110
11.0	170	6	22	354
16.0	84	10	26	270

Thus, the obtained results demonstrate that the proposed method for solution of inverse problems can be successfully applied to solve serious ecological problems. When developing specific techniques based on the proposed algorithm, it should be taken into account that, under meteorological conditions unfavorable for pollutant spread (wind velocity of 2 m/s accompanied by stable atmospheric stratification), the detected considerable increases of the pollutant concentration could rather be caused by pollutant accumulation in the surface atmospheric layer even at relatively low source power, than by instant emission.

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