Determination of parameters of a multi-point source of aerosol pollution by solving inverse problem

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The generation power of an ensemble of point-like stationary sources of atmospheric pollution is determined based on pollutants concentration measured at a series of control points. The problem is stated, the corresponding differential equations are derived, and algorithms and difference schemes for their numerical solution are discussed. Test computations for a linear source have demonstrated a close agreement with the initial data for both homogeneous and inhomogeneous surfaces. The proposed approach was also applied to analysis of field experiments conducted with the help of an agricultural aircraft used as a linear source. The experiment imitated a combating against agricultural pests. The calculated coordinates and generation power of the source are compared with the actual values.

Introduction

When studying theoretically and experimentally ecological problems like environmental hazards of industrial emissions, it is often necessary to solve some inverse problems, such as determination of coordinates of unknown sources of atmospheric pollution and their intensity, using concentrations of impurities measured at a limited number of control points. For example, sometimes it is needed to determine the coordinates of a plant and the amount of pollutants emitted into the atmosphere at a hidden sudden blowout. Industrial plants are, as a rule, point-like sources. In other cases, practically important, a probable source is linear or planar (for example, land surface polluted with chemical or radioactive substances).

Classically, such problems are solved by iteration methods (steepest descent method, random-walk method, and others). In this case, at each step of iteration it is required to solve the direct problem of pollutant spreading. Computationally, this approach is very time-consuming, especially, if some pollutant spreads over significantly inhomogeneous surface and under complex meteorological conditions. Besides, with a poor choice of the initial approximation needed for the iteration process, one can lose a part of solution or even obtain some absolutely incorrect solution. The more productive and rigorous approach based on the solution of the problem conjugated with the semiempirical equation of turbulent diffusion was proposed by Marchuk and developed by his followers.[1–3] We have used this approach earlier for solution of inverse problems. Thus, in Ref. 4 the efficient and stable method was proposed by us for determining the coordinates and intensity of a point-like source of atmospheric pollution based on measuring the impurity concentrations at a limited number of control points. In this paper we propose to apply this approach to the case of a multi-point source. From the viewpoint of numerical solution of inverse problems, sets of point-like sources, approximating linear, planar, and other sources of complex configuration, can be treated as multi-point ones as well.

Statement of the problem

Let us consider a rectangular area Ω_0 $(0 \le x \le X,$ $0 \le y \le Y,\ 0 \le z \le H)$. The axis z is assumed a vertical coordinate, and H is the height of the atmospheric boundary layer. Assume that some area $\Omega \in \Omega_0$ contains a uniformly distributed pollution source, which forms a field of pollutant concentration c at some fragment S of the horizontal cross section at the altitude $z = h$. The letter S denotes also the area of this fragment. According to Refs. 1 and 4, the conjugate system of equations for the auxiliary function c^* has the form

$$-\frac{\partial c^*}{\partial t} - u\frac{\partial c^*}{\partial x} - v\frac{\partial c^*}{\partial y} - (w - w_s)\frac{\partial c^*}{\partial z} = \frac{\partial}{\partial x} k_x \frac{\partial c^*}{\partial x} + \frac{\partial}{\partial y} k_y \frac{\partial c^*}{\partial y} + \frac{\partial}{\partial z} k_z \frac{\partial c^*}{\partial z} + R^*$$

$$c^*\Big|_{t=0} = c^*\Big|_{x=0,\ X;\ y=0,\ Y} = c^*\Big|_{z=H} = 0, \qquad (1)$$

$$\left(k_z \frac{\partial c^*}{\partial z} + 2w_s c^*\right)\Bigg|_{z=0} = \beta\, c^*\Big|_{z=0},$$

where t is the time; u, v, and w are mathematical expectations of the wind velocity components; w_s is the rate of sedimentation of pollutant particles; k_x, k_y, and k_z are the coefficients of turbulent diffusion in the direction of the corresponding axes; β is the constant of interaction of pollutant particles with the surface; R^* is some function whose specific form will be presented below. The key property of the method of solution of conjugate problems consists in the integral identity[1,4]:

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$$\int_0^T \int_{\Omega_0} R^* \, c \, \mathrm{d}\Omega \, \mathrm{d}t = \int_0^T \int_{\Omega} R \, c^* \, \mathrm{d}\Omega \, \mathrm{d}t, \quad (2)$$

where T is the period of time during which the solution is sought; c is the result of solution of the semiempirical equation of turbulent diffusion with the right-hand side $R = R(x, y, z, t)$ describing a presence of sources and sinks of the pollutant. Let us assume $R = \begin{cases} R_0 \, \delta(t); & x, y, z \in \Omega \\ 0; & x, y, z \notin \Omega \end{cases}$ and set R^* in the form

$$R^* = \begin{cases} \frac{1}{S} \delta(x - \xi, y - \eta, z - h); & \xi, \eta \in S \\ 0; & \xi, \eta \notin S \end{cases}.$$

Upon solution of the conjugate problem (1), we can find c^* and, according to Eq. (2), obtain

$$\frac{1}{S} \int_0^T c(\xi, \eta, h, t) \, \mathrm{d}t =$$

$$= \int_{\Omega} R \left(\int_0^T c^* \, (x, y, z, \xi, \eta, h, t) \, \mathrm{d}t \right) \mathrm{d}\Omega. \quad (3)$$

Upon introduction of the auxiliary variables

$$D = \frac{1}{S} \int_0^T c \, \mathrm{d}t; \quad D^* = \int_0^T c^* \, \mathrm{d}t,$$

Eq. (3) takes the form

$$D(\xi, \eta, h) = R_0 \int_{\Omega} D^*(x, y, z, \xi, \eta, h) \, \mathrm{d}\Omega, \quad (4)$$

where $D(\xi, \eta, h)$ is the time-integral pollutant concentration at some point (ξ, η, h) on the plane S. It follows herefrom that at given $D(\xi, \eta, h)$ and S the minimum of the functional

$$J = \int_S \left| R_0 - \frac{D(\xi, \eta, h)}{D^*(x, y, z, \xi, \eta, h)} \right| \mathrm{d}S \quad (5a)$$

estimates the sought area Ω. Note that in order to find this area, it is not necessary to know the solution of the direct problem of spreading, but it is sufficient to know only c^* and $D(\xi, \eta, h)$, which is interpreted as some measured integral concentration at the area S.

Results of numerical experiments and their analysis

The problem (1) was solved by the finite-difference method with the use of the procedure of splitting by physical processes and spatial variables. The applied difference schemes were constructed taking into account dual representation of the functionals (2) under study. The methodology of constructing the difference analog to the conjugate problem was considered by Marchuk in Ref. 1. In this case, the functional (5a) at nodes of the computation difference grid takes the form

$$J = \sum_{m=l}^{M} \left(\frac{| \bar{R} - R_{0,m} | \; R_{0,m}}{\bar{R}} \right), \quad (5b)$$

where

$$R_{0,m} = \frac{D(\xi_m, \eta_m, h)}{\sum_{n=1}^{N} D^*(x_n, y_n, z_n; \xi_m, \eta_m, h)}; \quad \bar{R} = \frac{1}{M} \sum_{m=l}^{M} R_{0,m}$$

$(x_n, y_n, z_n) \in \Omega$; $(\xi_m, \eta_m) \in S$; $n = \overline{1, N}$; $m = \overline{1, M}$.

The algorithm considered above was tested both in model computations and with the use of experimental data on pollutant spreading in the atmosphere.

The model computations included a solution of the direct problem of pollutant spreading from a given source. The concentration calculated at some pre-chosen points was taken as "measured data," and then these data were used to reconstruct the characteristics of the source by the above algorithm. For computations, we took a flat plate with homogeneous and inhomogeneous characteristics of the surface. The fields of meteorological elements were determined with the use of a numerical-analytical model.[6] We chose a linear uniformly distributed source. Having performed a cycle of computations, we found that the power of a linear source was reconstructed accurate to 3–5%, and the coordinates of the source were reconstructed accurate to one step of the computation scheme.

It is more interesting and practically important to check this method using actual data of field measurements. For this purpose, we used the experimental results from Ref. 7. Let us consider the experiment carried out at 16:30 L.T. on October 4, 1988, above a thermally and orographically homogeneous area near Novosibirsk. The scheme of the experiment is shown in Fig. 1. A preparation in amounts of 400 kg was sprayed from AN–2 agricultural aircraft flying at the altitude of 50 m. It is well-known that such an experimental scheme simulates an instantaneous linear aerosol source in the atmosphere. The wind speed along the axis x was 4 m/s at the altitude of 4 m. Table 1 gives the time-integral concentrations measured at a number of points.

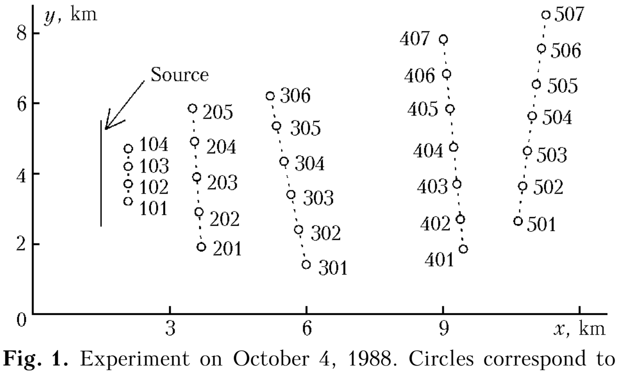

Fig. 1. Experiment on October 4, 1988. Circles correspond to sampling points; an arrow shows the line of the preparation spraying.

Table 1. Integral concentration of the preparation measured in the experiment on October 4, 1988 (in mg/(m^3·s))

Point	Measured concentration	Point	Measured concentration
101	0	401	23.50
102	32.31	402	18.18
103	33.15	403	9.62
104	59.58	404	0
201	70.49	405	0
202	13.51	406	0
203	0.13	407	0
204	43.64	501	1.93
205	3.08	502	3.66
301	5.85	503	4.34
302	88.11	504	7.52
303	36.64	505	0.76
304	13.85	506	0.09
205	18.74	507	0.08
306	15.10	–	–

Solving the inverse problem, we reconstructed the following parameters of the linear source: coordinates of the initial point, the length of the spraying line, and the mass of the sprayed substance. It was assumed that the aircraft flew along the axis y. Because of the atmospheric turbulence, errors in the input parameters, and other uncontrolled factors, it is worth speaking about some area, rather than point, containing the minimum of the functional (5b). This area is characterized by the initial point of the aircraft motion $(\bar{x}, \bar{y}, \bar{z}) = \frac{1}{N_0}\left(\sum_{n=1}^{N_0} x_n, \sum_{n=1}^{N_0} y_n, \sum_{n=1}^{N_0} z_n\right)$, the characteristic linear scale $\bar{\Lambda} = \frac{1}{N_0}\sum_{n=1}^{N_0} \Lambda_n$ corresponding to the length of the spraying line, and the mass of the emitted substance $\bar{Q} = \sum_{n=1}^{N_0} Q_n$, where N_0 is the number of the first minima of the functional (5b) with the corresponding values of the spraying line length and mass of the emitted substance Λ_n and Ω_n. The computations have shown that the optimal value of N is roughly equal to 50.

Table 2 presents the reconstructed characteristics of the linear source for the experiment conducted on October 4, 1988. These values were obtained based on the data on the concentrations from the first measurement column, first–second columns, first–third columns, and so on. The comparison of the obtained data with the actual parameters of the source demonstrates their close agreement. The only exclusion is the results obtained by the data from the first measurement column. This can be explained by several reasons, for example, rough approximation nearby the source, neglect of aircraft contrail, and some others. It should be also emphasized that in spite of wide scatter of experimental data (for example, by two to three orders of magnitude in the second column) the source parameters were reconstructed rather well. The maximum relative error in determination of the mass of the emitted substance did not exceed 60%, and the horizontal coordinates of the source were determined, as a rule, accurate to one step of the used difference grid.

The method was also tested with a limited number of measuring points. Table 3 presents the results of such numerical experiments. The first row of this table lists the numbers of measuring points, which were used in computations. As is seen from Table 3, the source parameters in this case are reconstructed somewhat worse than in the case of all measuring points. However, when four points are used, the results improve.

Table 2. Parameters of the pollution source reconstructed based on the data of the experiment on October 4, 1988

Parameter	Results obtained using the data of the following sampling columns					Actual value
	1	1–2	1–3	1–4	1–5	
$\bar{\Lambda}$, km	2.65	3.50	3.50	3.50	3.50	3.50
$\bar{x}$, km	1.90	1.20	1.20	1.30	0.80	1.50
$\bar{y}$, km	2.80	2.00	2.00	2.00	2.00	2.50
$\bar{z}$, m	7	38	54	47	74	50
$\bar{Q}$, kg	22	206	358	326	592	400

Table 3. Parameters of the source reconstructed using a limited number of measuring points

Parameter	Results obtained using the data at the following sampling points			Actual value
	201, 302	201, 302, 401	201, 302, 401, 504	
$\bar{\Lambda}$, km	3.00	2.95	3.80	3.50
$\bar{x}$, km	2.20	2.20	2.00	1.50
$\bar{y}$, km	1.50	1.60	1.80	2.50
$\bar{z}$, m	93	49	54	50
$\bar{Q}$, kg	525	294	397	400

Conclusion

The algorithm based on the method of conjugate equations is justified as applied to determination of parameters of a multi-point source of atmospheric pollution. The algorithm uses as the initial data the pollutant concentrations measured at some control points. The theoretical results of this work generalize the approach we used earlier to find characteristics of a point-like source.[4] To demonstrate its capabilities, we used the proposed method in computations involving actual experimental data. The obtained results are indicative of rather good reconstructibility of the coordinates, size, and power of the source. The proposed algorithm has considerable promise and can be successfully used in a wide variety of ecological problems.

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