Taking account of dispersion of measured concentration values in the problems of searching for latent sources of atmospheric aerosol pollutants

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The inverse problem of finding the characteristics of latent sources of atmospheric aerosol pollutants based on monitoring data is considered. When solving such problems, the measured values of the pollutant concentration in the general case differ from their mathematical expectations. The data dispersion is due to the statistical nature of the process of atmospheric pollutant propagation and the presence of measurement errors. We propose a method for taking account of dispersion of the measured concentration values. We also determine the probability of falling the unknown source of impurity in a given region and lying its power in a given range of values.

Working out of economical and stable methods for solving the inverse problems, when it is required to find the type, coordinates, and power of pollutant sources based on the information about the concentration of pollutants measured at a limited quantity of reference points, is a very important and urgent practical task. It is conditioned by the necessity of searching for latent sources of atmospheric pollution appearing at technogenic failures and industrial emissions of impurities.

We have $proposed^{1-3}$ an effective method for solving such problems based on the use of the equation conjugate to a semiempirical equation of the turbulent diffusion. As a result of a joint consideration of direct and inverse problems, a functional was derived, which connects the unknown characteristics of a pollutant source, the measured concentration values, and the sensitivity function, which is a solution of the conjugate equation. The minimum of this functional determines the sought characteristics of the source. In this case it is assumed that the mathematical expectations of concentration are used as input values and the instrumental measurement errors are absent. However, the measured values of pollutant concentration generally do not coincide with the mathematical expectations of concentration and have a scatter due to the statistical nature of the process of the atmospheric pollution spread and the presence of measurement errors.

This paper describes a method of taking account of the spread of the measured concentration values when solving inverse problems. We determine the probability that unknown pollutant source is in a given region and its power is in a given range of values.

Let C_i be the mean concentration for the time interval [0, T] measured at the *i*th reference point, which, as it was noted above, generally differs from the mathematical expectation of the concentration value. Let $\varphi_i(C_i)$ be the known function of the probability density of the measured concentration value. According to the algorithm of the inverse problem solution, we sequentially solve the conjugate equation under corresponding initial and boundary conditions for each reference point *i*, using the measured value C_i ; and calculate theoretically possible values of the source power Q_{ki} at each *k*th node of the difference grid. The impurity concentration depends linearly on the power of the pollutant source. Therefore, the calculated values of Q_{ki} can be described by the analogous function of the power probability density $\varphi_{ki}(Q_{ki})$.

For definiteness. consider two-parameter functions of the probability density with the given values of mathematical expectation and variance. At each point of space we calculate the standard deviation of the power σ_{qki} , connected with the corresponding standard deviation of the concentration σ_{ci} by the relationship $\sigma_{qki} = \sigma_{ci} Q_{ki} / C_i$. Thus, at each kth point of space we have I pairs of values of Q_{ki} and σ_{qki} (I is the number of reference points, at which the concentrations are measured). Let (Q_{\min}^{κ}) , Q_{\max}^{R}) be the common region of intersection of all the above-mentioned intervals (see Fig. 1). Then it is evident that

$$P_{k} = \min_{i} \left(\int_{Q_{\min}^{k}}^{Q_{\max}^{k}} \varphi_{ki}(Q) \, \mathrm{d}Q \right)$$

is the probability of the fact that there is a source at the *k*th point of space, whose power falls in the region (Q_{\min}^k, Q_{\max}^k) , and which produces at the *i*th reference points the concentration, whose mathematical expectation falls in the range $C_i \pm \sigma_{ci}$.



Fig. 1. An example of the variation of values of the source power for three reference points of the concentration measurement.

To test the above-mentioned approach, two series of calculations were performed. In the first series we used the theoretically calculated values of the concentration obtained by solving the direct problem. These values were interpreted as experimental and used further for solving the inverse problem. A large body of results have shown that for the case $\sigma_{ci} = 0$, when the measured concentration values are strictly equal to the mathematical expectations, the calculated values of the source parameters (power and coordinates) coincide with the true values.

To account for the concentration measurement errors, two variants of setting σ_{ci} were considered. In the first variant the relative error $\delta_c = \sigma_{ci}/C_i$ was set the same at all reference points. In the second variant it was different at different reference points. Further, using the above algorithm, the inverse problem was solved and the probability of the source location at an arbitrary point of space was calculated.

Table 1 shows the results of calculations. The values of the concentration relative error at three reference points δ_c , the considered concentration error interval ΔC , the calculated values of the source coordinates, the minimal Q_{\min}^k and maximal Q_{\max}^k values of power, and the probability P of this event are presented.

 Table 1. Results of calculations for equal concentration measurement errors at the reference points

#	$\delta_c, \%$	ΔC	$x_0, y_0,$ km, z_0 , m	Q_{\min}^k , arb. units	Q_{\max}^k , arb. units	Р
1	10; 10; 10	$2\delta_{ci}$	4; 3; 50	0.90	1.10	0.68
2	10; 10; 10	$4\delta_{ci}$	4; 3; 50	0.80	1.20	0.95
3	10; 10; 10	$6\delta_{ci}$	4; 3; 50	0.70	1.30	0.99
4	50; 50; 50	$2\delta_{ci}$	4; 3; 50	0.50	1.50	0.68
5	50; 50; 50	$4\delta_{ci}$	4; 3; 50	0.00	2.00	0.95

Note. True values of the source parameters are: $x_0 = 4 \text{ km}, y_0 = 3 \text{ km}, z_0 = 50 \text{ m};$ the power equals 1 arbitrary unit.

It is seen that the probability maximum is always at the point where the source is located. The increase of the error standard deviation (see calculations 1, 4 and 2, 5) results in the increase of the range of the possible power values; i.e., the error of the power determination increases at a fixed value of the probability of falling the power in this range. The range of power variation, i.e., its error, is always proportional to the concentration measurement error. The increase of the considered range of the concentration variation ΔC (see calculations 1–3 and 4, 5) also increases the range of the power variation and the probability of the power location in this range. The calculational results corresponding to the second case (the concentration measurement errors are different at different reference points), are given in Table 2. Relative errors of the concentration δ_c at the reference points are presented. Then the coordinates are given of the point, at which the maximal probability is observed. The last three columns contain the minimal Q_{\min}^k and the maximal Q_{\max}^k values of the source power and the probability *P* of this event, respectively.

 Table 2. The calculation results for different concentration measurement errors at the reference points

#	Values of δ_c (%) at points with numbers) at bers	$\begin{array}{c} x_0, \ y_0, \\ \mathrm{km}, \end{array}$	Q_{\min}^k	Q_{\max}^k	Р
	1	2	3	4	5	6	z_0, m	ard, units	ard. units	
1	50	30	40				4; 3; 10	0.73	1.35	0.68
2	50	30	40	20			5; 3; 50	0.80	1.18	0.46
3	50	30	40	20	10		4; 3; 10	0.97	1.19	0.23
4	50	30	40	20	10	5	4; 3; 10	1.01	1.12	0.11
5		30	40	20	10	5	4; 3; 10	1.01	1.12	0.13
6			40	20	10	5	4; 3; 10	1.01	1.12	0.13
7				20	10	5	4; 3; 80	1.02	1.12	0.28
8				40	20	10	4; 3; 100	1.04	1.27	0.31
9				50	30	40	4; 3; 90	0.74	1.37	0.68

Note. True values of the source parameters see in Table 1.

It is seen that the sequential addition of reference points with decreasing errors of the concentration measurement (see the calculations 1-5) reduces the range of possible values of the source power, i.e., the accuracy of the source power determination increases, but the probability of finding the source of such power at a given point decreases. Analysis of the probability field indicates that in this case the region of the possible detection of the source at a given probability value also decreases, i.e., the accuracy of determination of the source coordinates increases.

The successive addition of reference points with increasing errors of the concentration measurement (see, the calculations 4–7) does not change the range of the possible value of the source power, but decreases the probability of this event. At the same number of reference points (see the calculations 7, 8 or 8, 9) the decrease of the concentration measurement error increases the accuracy of the source characteristic determination, but decreases the probability of this. Evidently, in the general case a singular "principle of uncertainty" is true: the more precisely the source characteristics are determined, that corresponds to the increase in the concentration measurement accuracy and the number of reference points, the less is the probability of this event.

In the second series of calculations we used the experimental data obtained during developing the aerosol technology of plant protection against the insects pests⁴ and when studying the effect of the Berdsk Chemical Plant emissions on the atmosphere of the surrounding development land.⁵ As for the theoretical data, two variants were considered. For the first variant, it was assumed that the measurement errors were absent and the measured experimental values of the concentration at the reference points coincided with the mathematical expectation. As it was shown in Ref. 3, in this case the mean error in the determination of the source coordinates with the use of data from Ref. 4 was 83 m, and the standard deviation of coordinates was 70 m. The corresponding values for the calculated source power were 89 and 96%. It should be noted that the size of the experimental area was equal to 5×5 km, the measured concentration values include the instrumental error, and the concentration value itself is of the random character due to the atmospheric turbulence. For example, at certain neighboring reference points being well off the source and separated by 50 m, the concentration values varied from 2.5 to 5 times.

The same results were obtained with the experimental data from Ref. 5. In that case, the mean error in determination of the source coordinates was equal to 557 m, and its standard deviation was 360 m. Corresponding values for the source power were 38 and 28% at the size of the experimental area of 4.6×4.4 km.

Significant errors in determination of the source coordinates in the experiments in Ref. 5 as compared to Ref. 4, in our opinion, depend on the fact that the formers were carried out under field conditions with relatively homogeneous underlying surface, whereas the latter ones were conducted under urban conditions with inhomogeneous underlying surface. Note that in the used procedure, reconstructing the field of velocity and turbulence in the atmospheric boundary layer based on the meteorological information, the city building is taken into account through setting a corresponding parameter of roughness, and the air circulation and pollution spread near individual buildings is not modeled.

In the second case, when using the same experimental data, it was assumed that the measured concentration values differed from the mathematical expectation and were described by the lognormal distribution law. It was also assumed that the relative measurement error was the same at all reference points. Figure 2 presents the results of these calculations for the 5% standard deviation of the logarithm of the experimental concentration value with the use of data from Ref. 4.

With regard to the above-mentioned comment about the concentration measurement errors, the agreement between the calculated and experimental values of the source characteristics may be considered satisfactory. Similar results were obtained when using data from Ref. 5.



Fig. 2. Results of reconstruction of the source parameter values according to data from Ref. 4. The location of the source is denoted by a cross. Isolines numbered 1-3 correspond to the probability values P = 0.1; 0.3; 0.5.

Thus, the results of the given calculations make it possible to take into account the statistical nature of the atmospheric spread of pollutants and the errors in measuring their concentration when solving the inverse problems of spreading the atmospheric contaminants.

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