Determination of total intensity of stationary point sources of atmospheric pollutants by the method of maximal likelihood

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In this paper, intensities of an ensemble of point stationary sources of atmospheric pollutants are determined by values of pollutant concentration measured in several test points. To find the sought characteristics, the method of maximal likelihood was applied. The likelihood function was plotted on the base of results obtained earlier in the authors' study of atmospheric pollutants' concentration. The calculations were performed for a flat underlying surface situated at the latitude of Novosibirsk city. The values of pollutant concentration obtained in solving the "direct" propagation problem were taken as the "measured" values of concentration. According to calculations, this approach turns to be efficient for a rather complicated "inverse" problem.

Introduction

Let a number of point stationary sources act in a certain domain of the space. To describe aerosol propagation from the sources in the boundary layer of the atmosphere, we'll use a model based on the semi-empirical equations[8]

$$\sum_{r=1}^{3}\left(U_r \frac{\partial \bar{C}}{\partial x_r} - \frac{\partial}{\partial x_r}\sum_{s=1}^{3} K_{rs}\frac{\partial \bar{C}}{\partial x_s}\right) = Q; \qquad (1)$$

$$\sum_{r=1}^{3}\left(U_r \frac{\partial \sigma^2}{\partial x_r} - \frac{\partial}{\partial x_r}\sum_{s=1}^{3} K_{rs}\frac{\partial \sigma^2}{\partial x_s}\right) = 2\sum_{r=1}^{3}\sum_{s=1}^{3} K_{rs}\frac{\partial \bar{C}}{\partial x_r}\frac{\partial \bar{C}}{\partial x_s} - \frac{\varepsilon}{Rb^2}\sigma^2, \qquad (2)$$

where $\bar{C}$ and σ^2 are mathematical expectation of concentration and its dispersion, respectively, U_r are the components of mathematical expectation of the field of wind velocity, K_{rs} are the components of the tensor of turbulent diffusion coefficients, Q describes the sources of admixture, b^2 is kinetic energy of turbulence, ε is its dissipation rate, R is the empirical constant.[8]

Let the sources' coordinates x_i, y_i, z_i, $(i = \overline{1, m})$ be known. Let the intensity of each source be assigned the form $q_i = \lambda_i q_0$ where q_0 is a unity value of intensity, λ_i are dimensionless constants. Let the observation points be situated within the chosen area at the points x_j, y_j, z_j, $(j = \overline{1, n})$ where average values of harmful admixtures' concentration C_{avj} are detected. As a rule, measurements of admixture concentration are realized by averaging of its instant values $C(t)$ by a certain finite time interval T:

$$C_{av} = \frac{1}{T}\int_0^T C(t_1)\,dt_1. \qquad (3)$$

Owing to this, C_{av} is a random value as a function of a random variable. It is well-known that this estimate is unbiased and its dispersion is (see, for instance, Ref. 10)

$$\sigma_{av}^2 = 2\,\sigma^2\frac{1}{T}\int_0^T\left(1 - \frac{t_1}{T}\right) r(t_1)\,dt_1, \qquad (4)$$

where $r(t)$ is the normalized correlation function of concentration pulsation. As $T \to \infty$, sample values C_{av} tend to mathematical expectation of concentration $\bar{C}$, and dispersion σ_{av}^2 tends to zero.

Solving Eq. (1), one can obtain mathematical expectations C_{avj}, namely, values of $\bar{C}$, by assuming

$$Q = \sum_{i=1}^{m}\lambda_i\,q_0\,\delta(x - x_i)\,\delta(y - y_i)\,\delta(z - z_i),$$

where $\delta(...)$ is the Dirac delta. The equation (1) is linear. So one write

$$\bar{C}_j = \sum_{i=1}^{m}\lambda_i\,\bar{C}_{ij}, \qquad (5)$$

where $\bar{C}_{ij}$ are solutions of the equation (1) for $Q = q_0\,\delta(x - x_i)\,\delta(y - y_i)\,\delta(z - z_i)$ (the solutions are taken in the jth point). Similarly we obtain that

$$\sigma_j^2 = \sum_{i=1}^{m}\lambda_i^2\,\sigma_{ij}^2, \qquad (6)$$

where σ_{ij}^2 are solutions of the equation (2) which are taken at the jth point and correspond to the values $\bar{C}_{ij}$ obtained by Eq. (1).

This paper deals with the problem of determining weight coefficients λ_i, i.e., determining intensity of pollutant sources by observation data on concentration and additional information obtained from the solution of the equations (1) and (2) for sources of unity intensity. The problem that was formulated above belongs to the class of "inverse" problems. Classical approaches to its solution are based on equations adjoint to the semi-empirical equation of turbulent diffusion (1).[6] Below we consider a variant of the solution of this problem. It uses the statistical nature of the process of pollutant propagation in the atmosphere.

Methods

To determine the coefficients λ_i, which also are random values in the general case, we apply the method of maximal likelihood.[10] Let us introduce an *a priori* probability density of the estimated parameters $p_{pr}(\lambda_i)$. It is an unknown value. Let the probability density of the observed mean concentration values is $p(C_{\text{av}j}|\lambda_i)$ for fixed parameters λ_i. By the multiplication theorem, the joint probability density of $C_{\text{av}j}$ and λ_i is

$$p(\lambda_i|C_{\text{av}j}) = p_{pr}(\lambda_i)\, p(C_{\text{av}j}|\lambda_i) = p(C_{\text{av}j})\, p(\lambda_i|C_{\text{av}j}).$$

Owing to this, we obtain the classical formula for the conditional probability density λ_i for a given sample of the values $C_{\text{av}j}$

$$p(\lambda_i|C_{\text{av}j}) = \frac{p_{pr}(\lambda_i)\, p(C_{\text{av}j}|\lambda_i)}{p(C_{\text{av}j})}\,.$$

This value is the posterior conditional probability density $p(\lambda_i|C_{\text{av}j}) = p_{ps}(\lambda_i)$. The conditional probability density $p(C_{\text{av}j}|\lambda_i)$ considered as a function of λ_i is said to be the likelihood function $p(C_{\text{av}j}|\lambda_i) = L(\lambda_i)$. If the posterior probability density is of a rather "good" form, namely, if it is unimodal and almost symmetric, it is natural to seek an estimate of the parameters λ_i that has minimal posterior variance. The set of values that provides the maximal value of the posterior probability density for given $C_{\text{av}j}$ is taken as an estimate for λ_i in the method of maximal likelihood. In some cases, it seems to be convenient to seek solutions of the system of equations[10]

$$\frac{\partial}{\partial \lambda_i} \ln L(\lambda_i) = 0; \quad i = \overline{1,\, m}, \tag{7}$$

which explicitly depend on the sample $C_{\text{av}j}$.

Now let us begin to construct the likelihood function $L(\lambda_i)$. For the considered problem, it is natural to assume that every pairs of values $C_{\text{av}j_1}$ and $C_{\text{av}j_2}$ are statistically independent for $j_1 \neq j_2$ and $p_j(C_{\text{av}j}|\lambda_i) \neq 0$. Then

$$L(\lambda_i) = \prod_{j=1}^{n} p_j(C_{\text{av}j}|\lambda_i), \tag{8}$$

where $p_j(C_{\text{av}j}|\lambda_i)$ is the probability density for the observation of the mean concentration value $C_{\text{av}j}$ for fixed λ_i at the jth point.

Let us take Eq. (5) as a parametric estimate of the mathematical expectation of $C_{\text{av}j}$. For the parametric estimation of dispersion of $C_{\text{av}j}$, let us suppose that the correlation function in Eq. (4) has the exponential form $r(t) = \exp(-|t|/\tau_e)$ where τ_e is the Eulerian temporal scale of pollutant concentration pulsation. Then

$$\sigma_{\text{av}}^2 = \frac{2\,\sigma^2\,\tau_e^2}{T^2}\left[\frac{T}{\tau_e} - 1 + \exp(-T/\tau_e)\right]. \tag{9}$$

The probability density of the random value $C_{\text{av}j}$ is obtained theoretically and verified experimentally in Ref. 1:

$$p_j(C_{\text{av}j}|\lambda_i) = [1 - \text{erf}(\beta_{0j})]\,\delta(C_{\text{av}j}) + \frac{1}{\sqrt{\pi}\,\beta_j}\times$$

$$\times\left\{\exp\left[-\left(\frac{C_{\text{av}j} - \bar{C}_j}{\beta_j}\right)^2\right] - \exp\left[-\left(\frac{C_{\text{av}j} + \bar{C}_j}{\beta_j}\right)^2\right]\right\};$$

$$\beta_{0j} = \frac{\bar{C}_j}{\beta_j}\,, \tag{10}$$

where erf(...) is the error integral, β_j is the second parameter of the probability density function. It is connected with the variance $\sigma_{\text{av}j}^2$ by the relation

$$\frac{\sigma_{\text{av}j}^2}{\bar{C}_j^2} = \text{erf}(\beta_{0j})\left(1 + \frac{1}{2\,\beta_{0j}^2}\right) - 1 + \frac{1}{\sqrt{\pi}\,\beta_{0j}}\exp(-\beta_{0j}^2). \tag{11}$$

In Eq. (10), the term with the delta function describes the probability to observe zero values of $C_{\text{av}j}$, so it can be omitted for the considered problem.

Thus, the function of maximal likelihood can be assigned if and only if we know mathematical expectations of concentration $C_{\text{av}j}$ and variance $\sigma_{\text{av}j}^2$ at every jth point and the Eulerian temporal scale τ_e. Let us consider the results of some of our numerical experiments.

Results of calculations and their analysis

The calculations were performed for a plane underlying surface situated at the latitude of Novosibirsk. Thermal stratification of the atmosphere corresponded to conditions typical for summer at 15 h of local time in the Western-Siberian region. Thermal properties of the underlying surface were taken as characteristic for forest steppe. The calculations were performed within a rectangle parallelepiped with base $x = 34$ by $y = 42$ km. The y axis was directed to the north. The vertical coordinate was bounded by the height of the boundary layer of the atmosphere. The

Eulerian temporal scale was taken to be $\tau_e = 100$ s; $T = 30$ min.

Mean values of wind velocity components and temperature were calculated by the numerical–analytical technique.[5] For this purpose, wind velocity was taken to be 2 m/s at the height of 10 m. The wind blew in the direction of the x axis. Cloudiness was supposed to be absent. The obtained fields of wind velocity and temperature were used to assign K_{rs}, b^2, and ε. These characteristics, which are necessary for the solutions of the equations (1) and (2), were determined by the algebraic model described in Ref. 9. Here we used the hypothesis that K_{rs} are proportional to the corresponding components of the Reynolds viscous stress tensor. Experimental verification of the hypothesis was found earlier[2] in field conditions. The equations (1) and (2) were solved by numerical methods.[7] In the boundary condition for concentration on the underlying surface, the rate of particles' sedimentation was assumed to be $2\cdot10^{-2}$ m/s. The boundary condition for variance on the underlying surface was taken in accordance with Ref. 3. Concentration values obtained in such a way were considered as "measured," and then they were used to construct the likelihood function. The maximum values of $L(\lambda_i)$ and their corresponding values of λ_i were found by exhaustion.

In the first series of calculations, intensities of two sources were reconstructed. The scheme of their location and "measurement" points are presented in Fig. 1*a*. The results of calculations, together with the coordinates of the sources and "measurement" points, are presented in Table 1. The height of the points was always taken to be 25 m. In the first variant of calculations, intensity of the second source was varied. As seen from the data of Table 1, intensities of the two sources are reconstructed satisfactorily by four points up to the moment when their intensities begin to differ almost by three orders of magnitude. In the second variant of calculations, the height of the second source was decreased by two folds. The results of intensity reconstruction appear to be similar. In the third variant, the number of "measurement" points was reduced to three. One can see that the decrease of intensity of the second source by almost two orders of magnitude also leads to quite satisfactory results. The data of the fourth variant of calculations demonstrate that not bad results can be obtained even with two "measurement" points. The results of the fifth variant of calculations demonstrate that the increase of the distance between the sources leads to satisfactory coincidence of given and reconstructed intensities.

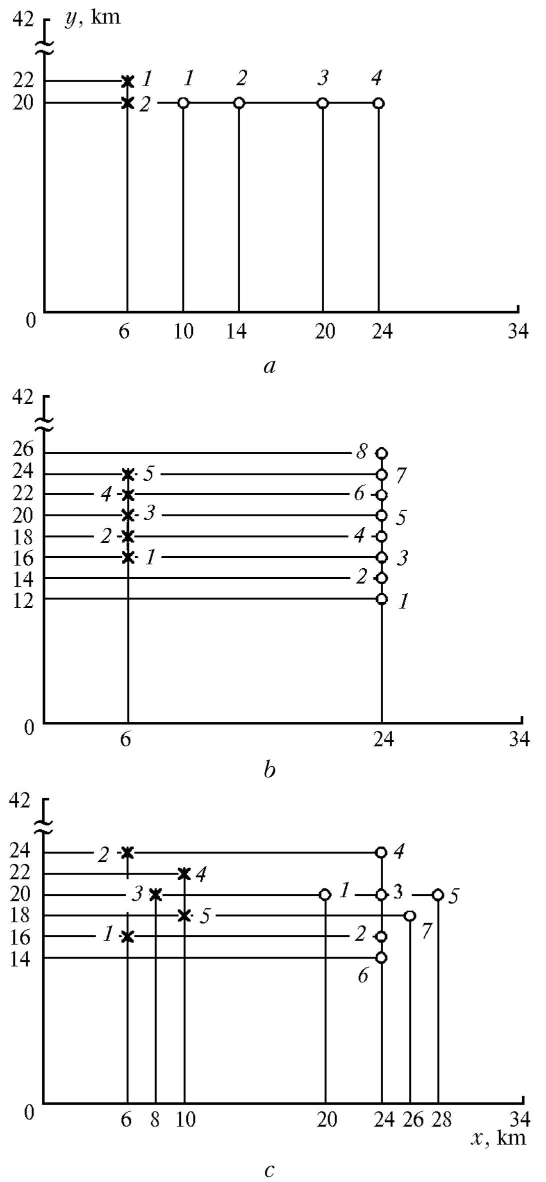

Fig. 1. Arrangement of pollutant sources (crosshairs) and points of concentration measurements (circles) within the calculation domain.

Table 1. Results of reconstruction of intensities for two sources (the first series of calculations)

Variant of calculations	Coordinates of the sources x, y (km); z (m)		Distance between the sources along the horizontal, km	Given/reconstructed intensity of the sources (conv. units)		Used points of concentration "measurement"			
	first	second		first	second	1	2	3	4
First	6, 20, 50	6, 22, 50	2	$10^{11}/10^{11}$	$10^{11}/10^{11}$	+	+	+	+
				$10^{11}/10^{11}$	$10^{10}/10^{10}$	+	+	+	+
				$10^{11}/10^{11}$	$10^{9}/10^{9}$	+	+	+	+
				$10^{11}/10^{11}$	$10^{8}/4\cdot10^{8}$	+	+	+	+
				$10^{11}/10^{11}$	$10^{7}/4\cdot10^{8}$	+	+	+	+

Variant of calculations	Coordinates of the sources x, y (km); z (m)		Distance between the sources along the horizontal, km	Given/reconstructed intensity of the sources (conv. units)		Used points of concentration "measurement"			
	first	second		first	second	1	2	3	4
Second	6, 20, 50	6, 22, 25	2	$10^{11}/10^{11}$	$10^{10}/10^{10}$	+	+	+	+
				$10^{11}/10^{11}$	$6\cdot 10^{9}/6\cdot 10^{9}$	+	+	+	+
				$10^{11}/10^{11}$	$4\cdot 10^{9}/3\cdot 10^{9}$	+	+	+	+
				$10^{11}/10^{11}$	$2\cdot 10^{9}/3\cdot 10^{9}$	+	+	+	+
				$10^{11}/10^{11}$	$10^{9}/5\cdot 10^{8}$	+	+	+	+
Third	6, 20, 50	6, 22, 50	2	$10^{11}/10^{11}$	$10^{10}/10^{10}$	+	+	+	−
				$10^{11}/10^{11}$	$8\cdot 10^{9}/8\cdot 10^{9}$	+	+	+	−
				$10^{11}/10^{11}$	$6\cdot 10^{9}/5\cdot 10^{9}$	+	+	+	−
Fourth	6, 20, 50	6, 22, 50	2	$10^{11}/10^{11}$	$10^{10}/10^{10}$	+	+	−	−
				$10^{11}/10^{11}$	$8\cdot 10^{9}/7\cdot 10^{9}$	+	+	−	−
Fifth	6, 18, 50	6, 24, 50	6	$10^{10}/9\cdot 10^{9}$	$10^{10}/10^{10}$	+	+	+	+
	6, 18, 50	6, 22, 50	4	$10^{10}/10^{10}$	$10^{10}/10^{10}$	+	+	+	+

Table 2. Results of reconstruction of intensities for five sources (the second series of calculations)

Given/reconstructed intensity of the sources (conv. units)					Used points of concentration "measurement"							
First	Second	Third	Fourth	Fifth	1	2	3	4	5	6	7	8
$5\cdot 10^{10}/5\cdot 10^{10}$	$5\cdot 10^{10}/5\cdot 10^{10}$	$5\cdot 10^{10}/5\cdot 10^{10}$	$5\cdot 10^{10}/5\cdot 10^{10}$	$5\cdot 10^{10}/5\cdot 10^{10}$	+	+	+	+	+	+	+	+
$5\cdot 10^{10}/5\cdot 10^{10}$	$5\cdot 10^{10}/5\cdot 10^{10}$	$5\cdot 10^{10}/5\cdot 10^{10}$	$5\cdot 10^{10}/5\cdot 10^{10}$	$5\cdot 10^{10}/5\cdot 10^{10}$	+	+	+	+	+	+	+	−
$5\cdot 10^{10}/5\cdot 10^{10}$	$5\cdot 10^{10}/5\cdot 10^{10}$	$5\cdot 10^{10}/5\cdot 10^{10}$	$5\cdot 10^{10}/5\cdot 10^{10}$	$5\cdot 10^{10}/5\cdot 10^{10}$	+	+	+	+	+	+	−	−
$5\cdot 10^{10}/5\cdot 10^{5}$	$5\cdot 10^{10}/5\cdot 10^{5}$	$5\cdot 10^{10}/4\cdot 10^{10}$	$5\cdot 10^{10}/8\cdot 10^{10}$	$5\cdot 10^{10}/9\cdot 10^{10}$	+	+	+	+	+	−	−	−
$5\cdot 10^{10}/5\cdot 10^{10}$	$5\cdot 10^{10}/4\cdot 10^{10}$	$5\cdot 10^{10}/8\cdot 10^{10}$	$5\cdot 10^{10}/8\cdot 10^{11}$	$5\cdot 10^{10}/9\cdot 10^{11}$	+	+	+	+	−	−	−	−
$5\cdot 10^{10}/4\cdot 10^{10}$	$5\cdot 10^{10}/10^{11}$	$5\cdot 10^{10}/2\cdot 10^{10}$	$5\cdot 10^{10}/2\cdot 10^{10}$	$5\cdot 10^{10}/2\cdot 10^{10}$	+	+	+	−	−	−	−	−

Table 3. Results of reconstruction of intensities for five sources (the third series of calculations)

Given/reconstructed intensity of the sources (conv. units)					Used points of concentration "measurement"						
First	Second	Third	Fourth	Fifth	1	2	3	4	5	6	7
$5\cdot 10^{10}/5\cdot 10^{10}$	$5\cdot 10^{10}/5\cdot 10^{10}$	$5\cdot 10^{10}/5\cdot 10^{10}$	$5\cdot 10^{10}/5\cdot 10^{10}$	$5\cdot 10^{10}/5\cdot 10^{10}$	+	+	+	+	+	+	−
$5\cdot 10^{10}/3\cdot 10^{10}$	$5\cdot 10^{10}/5\cdot 10^{10}$	$5\cdot 10^{10}/5\cdot 10^{10}$	$5\cdot 10^{10}/5\cdot 10^{10}$	$5\cdot 10^{10}/5\cdot 10^{10}$	+	+	+	+	+	−	−
$5\cdot 10^{10}/3\cdot 10^{10}$	$5\cdot 10^{10}/5\cdot 10^{10}$	$5\cdot 10^{10}/5\cdot 10^{10}$	$5\cdot 10^{10}/5\cdot 10^{10}$	$5\cdot 10^{10}/5\cdot 10^{10}$	+	+	+	+	−	−	−
$5\cdot 10^{10}/3\cdot 10^{10}$	$5\cdot 10^{10}/5\cdot 10^{10}$	$5\cdot 10^{10}/5\cdot 10^{10}$	$5\cdot 10^{10}/5\cdot 10^{10}$	$5\cdot 10^{10}/5\cdot 10^{10}$	+	+	+	−	−	−	−
$5\cdot 10^{10}/3\cdot 10^{10}$	$5\cdot 10^{10}/9\cdot 10^{9}$	$5\cdot 10^{10}/5\cdot 10^{10}$	$5\cdot 10^{10}/5\cdot 10^{10}$	$5\cdot 10^{10}/4\cdot 10^{10}$	+	+	−	−	−	−	−
$5\cdot 10^{10}/10^{11}$	$5\cdot 10^{10}/10^{11}$	$5\cdot 10^{10}/10^{11}$	$5\cdot 10^{10}/4\cdot 10^{10}$	$5\cdot 10^{10}/10^{11}$	+	−	−	−	−	−	−
$5\cdot 10^{10}/5\cdot 10^{10}$	$3\cdot 10^{10}/3\cdot 10^{10}$	$10^{10}/10^{10}$	$8\cdot 10^{9}/8\cdot 10^{9}$	$5\cdot 10^{9}/5\cdot 10^{9}$	+	+	+	+	+	+	+
$5\cdot 10^{10}/5\cdot 10^{10}$	$3\cdot 10^{10}/3\cdot 10^{10}$	$10^{10}/10^{10}$	$8\cdot 10^{9}/8\cdot 10^{9}$	$5\cdot 10^{9}/5\cdot 10^{9}$	+	+	+	+	+	+	−
$5\cdot 10^{10}/5\cdot 10^{10}$	$3\cdot 10^{10}/2\cdot 10^{10}$	$10^{10}/8\cdot 10^{9}$	$8\cdot 10^{9}/10^{9}$	$5\cdot 10^{9}/6\cdot 10^{8}$	+	+	+	+	+	−	−
$5\cdot 10^{10}/5\cdot 10^{10}$	$3\cdot 10^{10}/2\cdot 10^{10}$	$10^{10}/8\cdot 10^{9}$	$8\cdot 10^{9}/2\cdot 10^{9}$	$5\cdot 10^{9}/5\cdot 10^{8}$	+	+	+	+	−	−	−

The second series of calculations was performed for five sources arranged in a line. They simulated a linear source of a pollutant (see Fig. 1*b*). The number of "measurement" points by which the intensities were reconstructed was up to eight. They were also placed in a line. The reconstructed values of intensity are presented in Table 2. Good results are obtained in the case when we use from six to eight points. For less numbers of points, significant discrepancy with the given intensities is observed.

The third series of calculations was performed for five sources arranged irregularly and seven or less "measurement" points which were also arranged irregularly (see Fig. 1*c*). First, intensities of all the sources were assumed to be similar and the number of the "measurement" points varied. The data presented in Table 3 demonstrate that quite satisfactory results of intensity reconstruction for five sources can be obtained even with two "measurement" points. Other data presented in Table 3 correspond to the variant when intensities of an ensemble of five sources are different within the limits of an order of magnitude. We see that satisfactory results are obtained with five and more measurement points.

Conclusions

Thus, the results of calculations demonstrate that the method of maximal likelihood is efficient for the rather complicated "inverse" problem of reconstructing intensities of an ensemble of atmospheric pollutant sources. In the general case, as it is demonstrated by the above-mentioned results, it is necessary to optimize the number and arrangement of concentration monitoring points in accordance with the number of the sources and expected dispersion of intensities. The necessity to know not only pollutant concentration but also its variance is a non-trivial and complicating condition. Besides, it is important to match the period of concentration averaging with the Eulerian temporal scale of concentration pulsation. One can expect that the approach proposed in this paper can successfully complete classical (based on solving adjoint equations) methods of solving "inverse" problems.

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