

Errors in the emission rate estimated from solution of the inverse problem on the diffusion of an atmospheric pollutant

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When solving inverse problems, experimentally measured pollutant concentrations are usually used, but these values are subject to statistical scatter, which generally arises due to the turbulent nature of the pollutant diffusion process and due to measurement errors. In this paper we estimate the errors in determination of the emission rate of a pollution source. The practical examples presented demonstrate the importance of considering this factor in tackling specific tasks.

Diffusion of aerosol and gas pollutants in the atmosphere is usually described by two classes of problems. The first incorporates direct problems, when it is needed to find a pollutant concentration field from known source characteristics. The second class includes inverse problem, when it is needed to find the type, coordinates, and emission rates of pollutant sources from pollutant concentration measured at some control points. In the limits of Eulerian approach to description of the process of turbulent diffusion, the most fruitful method is the use of a semi-empirical equation²:

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

where \bar{C} and \bar{U}_i are the mathematical expectations of the pollutant concentration and wind velocity components; K_{ij} are the components of the tensor of turbulent diffusion coefficients (we assume $K_{ij} = 0$ at $i \neq j$); \bar{Q} is the term describing sources of pollution; $x = x_1$ and $y = x_2$ correspond to horizontal coordinates, and $z = x_3$ correspond to the vertical one; t is time. A bar denotes statistical averaging over an ensemble. Repeating subscripts mean summation. The direct problem is solved in the rectangular domain G with the surface S consisting of the lateral surface Σ , the lower base Σ_0 (at $z = 0$), and the upper base Σ_H (at $z = H$). The system of the initial and boundary conditions for Eq. (1) looks as follows:

$$\begin{aligned} \bar{C}(x, y, z, 0) = 0; \quad \bar{C} = 0 \quad \text{at } \Sigma, \Sigma_H; \\ -K_{zz} \frac{\partial \bar{C}}{\partial z} + V_s \bar{C} = \beta \bar{C} \quad \text{at } \Sigma_0, \end{aligned} \quad (2)$$

where V_s is the particle sedimentation rate; β is the parameter describing pollutant interaction with the surface.

An efficient method for solution of the inverse problems was developed by Marchuk.⁴ This method is

based on application of the equation conjugate to semi-empirical equation of the turbulent diffusion:

$$-\frac{\partial \bar{C}^*}{\partial t} - \frac{\partial \bar{U}_i \bar{C}^*}{\partial x_i} - \frac{\partial}{\partial x_i} K_{ij} \frac{\partial \bar{C}^*}{\partial x_j} = \bar{P}, \quad (3)$$

with the following system of the initial and boundary conditions:

$$\begin{aligned} \bar{C}^*(x, y, z, T) = 0; \quad \bar{C}^* = 0 \quad \text{at } \Sigma, \Sigma_H; \\ -K_{zz} \frac{\partial \bar{C}^*}{\partial z} + V_s \bar{C}^* = \beta \bar{C}^* \quad \text{at } \Sigma_0. \end{aligned} \quad (4)$$

Dual representation of the functional⁴

$$\int_0^T dt \int_G \bar{P} \bar{C} dG = \int_0^T dt \int_G \bar{Q} \bar{C}^* dG, \quad (5)$$

allows solution of a wide spectrum of inverse problems of pollutant diffusion.

In the theory of Marchuk's method, the solution of the direct problem (1) $\bar{C}(x_1, y_1, z_1, T)$ for

$$\bar{Q} = Q_0 \delta(x - x_0) \delta(y - y_0) \delta(z - z_0) \delta(t),$$

where x_0, y_0 , and z_0 are the coordinates of the pollution source, and Q_0 is the amount of the emitted substance (emission rate), and the solution of the inverse problem (3) $\bar{C}^*(x_0, y_0, z_0, 0)$ at

$$\bar{P} = \delta(x - x_1) \delta(y - y_1) \delta(z - z_1) \delta(t - T)$$

are of basic significance. In this case, according to Eq. (5),

$$\begin{aligned} \bar{C}(x_1, y_1, z_1, T; x_0, y_0, z_0, 0) = \\ = Q_0 \bar{C}^*(x_0, y_0, z_0, 0; x_1, y_1, z_1, T). \end{aligned} \quad (6)$$

The function \bar{C}_* determines the contribution of a unit-rate ($Q_0 = 1$) source located at the point x_0, y_0 , and z_0 and operated at $t = 0$ to the pollutant concentration at the point x_1, y_1, z_1 at the time $t = T$. The Green's function \bar{C}_* is usually called the sensitivity function.

The inverse problems are usually solved based on the use of experimentally measured pollutant concentrations that have some statistical scatter caused, generally, by the turbulent nature of the pollutant diffusion process¹ and by measurement errors. This paper is devoted to estimation of the errors in the emission rate of a pollutant source due to the factors mentioned above.

Let a pollutant source with the coordinates x_0, y_0 , and z_0 be operated at the time $t = 0$. In Ref. 3 we formulated the inverse problem of determining the coordinates of a pollutant source and considered some examples. Therefore, in this paper we believe that x_0, y_0 , and z_0 are known and dwell mostly on the problem of determining the unknown emission rate of a pollutant source through solution of the inverse problem. In the general case, the measured parameter is the integral concentration J which is a random variable:

$$J = \int_0^\infty C(t) dt, \tag{7}$$

where $C(t)$ is the instantaneous value of the pollutant concentration. Applying Eq. (7) to the operation of taking mathematical expectation, we obtain

$$\bar{J} = \int_0^\infty \bar{C}(t) dt. \tag{8}$$

Combining Eqs. (6) and (8), we have

$$\bar{J}(x_1, y_1, z_1) = Q_0 \int_0^\infty \bar{C}_* dt = Q_0 \bar{J}_*(x_0, y_0, z_0), \tag{9}$$

where \bar{J}_* is the sensitivity function of the integral pollutant concentration. We can see that the known mathematical expectation of the integral concentration \bar{J} and the solution of the conjugate equation \bar{C}_* allow the emission rate Q_0 of the source of atmospheric pollution to be determined. In solving particular problems, all terms of a statistical ensemble of the integral concentration and, consequently, the mathematical expectation are unknown. Therefore, in determining the source emission rate Eq. (9) usually includes the measured integral concentration J , in place of \bar{J} , rather than the ensemble-averaged one, namely,

$$Q_0 = J / \bar{J}_*. \tag{10}$$

The value of J is random, and this leads to the scatter in the estimated emission rate of the source. Consider first the distribution law of the estimated emission rate due to the statistical nature of the process of pollutant diffusion and then take into account the measurement error in concentration. As known,¹ the integral pollutant concentration has the following probability density function:

$$f_J(J) = \left[1 - \operatorname{erf} \left(\frac{\bar{J}}{\beta} \right) \right] \delta(J) + \frac{1}{\beta \sqrt{\pi}} \left\{ \exp \left[-\frac{(J - \bar{J})^2}{\beta^2} \right] - \exp \left[-\frac{(J + \bar{J})^2}{\beta^2} \right] \right\};$$

$$\frac{\sigma_J^2}{\bar{J}^2} = \operatorname{erf} \left(\frac{\bar{J}}{\beta_0} \right) \left(1 + \frac{\beta_0^2}{2\bar{J}^2} \right) - 1 + \frac{\beta_0}{\sqrt{\pi}\bar{J}} \exp \left(-\frac{\bar{J}^2}{\beta_0^2} \right), \tag{11}$$

where \bar{J} and β are the parameters of the function (11); σ_J^2 is the variance of J . According to Eq. (10), at the known solution of the inverse problem, the probability density function of the emission rate estimated by Eq. (10) coincides with Eq. (11) accurate to designations. It also follows from Eq. (10) that

$$\bar{Q}_0 = \bar{J} / \bar{J}_* \text{ and } \sigma_{Q_0}^2 = \sigma_J^2 / \bar{J}_*^2,$$

where $\sigma_{Q_0}^2$ is the variance of the found value of the emission rate. Thus, to specify the probability density function Q_0 , it is necessary to know the mathematical expectation of the integral pollutant concentration \bar{J} , its variance σ_J^2 , and the solution of the inverse problem \bar{C}_* .

The measurement errors in the integral pollutant concentration additionally contribute to the scatter of the estimated emission rate. In this case, in place of the instantaneous value of the integral concentration J , we observe other random value. Denote it as q . The estimation of the emission rate is similar to Eq. (10):

$$Q_0 = q / \bar{J}_*. \tag{12}$$

It follows from Eq. (12) that

$$\bar{Q}_0 = \bar{q} / \bar{J}_* \text{ and } \sigma_{Q_0}^2 = \sigma_q^2 / \bar{J}_*^2,$$

where σ_q^2 is the variance of the estimated emission rate taking into account instrumental errors.

Let $f(q, J)$ be the joint probability density of the measured parameter and the measured result. The parameters J and q are statistically dependent. Therefore, $f(q, J)$ can be written in the form⁶:

$$f(q, J) = h(q|J) f_J(J), \tag{13}$$

where $h(q|J)$ is the conditional probability density function of the measured value of the integral concentration q implying fixed measured J . Let us

write the obvious equation for the probability density function for the result measured

$$f_q(q) = \int_0^\infty h(q|J) f_J(J) dJ. \tag{14}$$

According to Eq. (12), the probability density function of the found value of the source emission rate allowing for the statistical scatter in the integral pollutant concentration and the measurement error coincides with Eq. (14) accurate to designations. In the further consideration, we believe that the conditional probability density function $h(q|J)$ is known. If the measurement technique is free of systematic errors, then $\bar{q} = \bar{J}$. To determine the variance of the measured value, calculate the second moment

$$\overline{q^2} = \int_0^\infty q^2 \int_0^\infty h(q|J) f_J(J) dJ dq = \int_0^\infty q^2 |_J f_J(J) dJ. \tag{15}$$

The conditional mathematical expectation of the squared q is¹:

$$\overline{q^2} |_J = s_q^2 + J^2,$$

where s_q^2 is the conditional variance of the measured integral concentration.

Then σ_q^2 can be presented as

$$\sigma_q^2 = \int_0^\infty s_q^2(J) f_J(J) dJ + \sigma_J^2. \tag{16}$$

In particular, it follows from Eq. (16) that with no measurement errors ($s_q^2 = 0$) the variance of q coincides with the variance of the measured integral concentration $\sigma_q^2 = \sigma_J^2$. For further analysis, let us specify the following model of the conditional probability density of the measured concentration:

$$h(q|J) = \frac{1}{q\rho\sqrt{2\pi}} \exp\left[-\frac{(\ln q - m)^2}{2\rho^2}\right];$$

$$\rho^2 = \ln\left(1 + \frac{s_q^2}{J^2}\right), \quad m = \ln J - \frac{1}{2}\rho^2. \tag{17}$$

We can see that the conditional mathematical expectation and the conditional variance of the measured integral concentration q calculated by Eq. (17) are equal to, respectively, J and s_q^2 . Consider two models of conditional variance of the measured result. In the first model it is assumed that $s_q^2 = \alpha_1^2 J^2$. Such a model describes the same contribution of measured values to the conditional standard deviation of the integral concentration normalized to J . In the second model

$s_q^2 = \alpha_2^2 J \bar{J}$. In this case, the measurement technique is assumed to be such that the contribution of measured values to the standard deviation of the integral concentration decreases in inverse proportion to the measured concentration.

For practical calculations, we should specify the variance of the integral pollutant concentration, which is determined by the following equation:

$$\sigma_J^2 = \int_0^\infty \int_0^\infty [C(t_1)C(t_2) - \bar{C}^2] dt_1 dt_2 =$$

$$= \int_0^\infty \int_0^\infty B_C(t_1, t_2) dt_1 dt_2, \tag{18}$$

where $B_C(t_1, t_2)$ is the correlation function of concentration fluctuations. We can see that σ_J^2 can be determined from double integration of the corresponding correlation function over time. Therefore, it sufficiently weakly depends on the specific form of $B_C(t_1, t_2)$. Based on this fact and on the peculiarities of the semi-empirical approach to description of turbulent diffusion, we proposed¹ the following quasi-stationary model of the correlation function:

$$B_C(t_1, t_2) = \sigma^2(t_1) \exp\left(-\frac{|t_2 - t_1|}{\tau}\right), \tag{19}$$

where τ is the Eulerian time scale of concentration fluctuations. Therefore,

$$\sigma_J^2 = 2\tau \int_0^\infty \sigma^2(t) dt. \tag{20}$$

As an example, let us consider pollutant diffusion from a source located in western suburbs of Novosibirsk (Fig. 1) situated on the banks of River Ob and shown by different grades of the gray scale (at the center of Fig. 1). The river shown by black divides the city into the right-bank and left-bank parts.

In computations we used meteorological conditions typical of a summer (July) day at the western wind with the speed of 3 m/s at the vane height. The source with a given emission rate was operated at 12:00 L.T. The wind velocity field over the city was determined with the use of the numerical-analytical model.² Then the semi-empirical equation (1) and the equation for the variance of the pollutant concentration were solved.⁶ Light isolines in Fig. 1 give the idea of the pollutant concentration field. Then the sensitivity function of the pollution source \bar{J}_* was determined by solving the conjugate equation (3). Points 1–3 in Fig. 1 served as measurement sites. The distribution function of the source emission rates calculated at these points neglecting measurement is shown in Fig. 2.

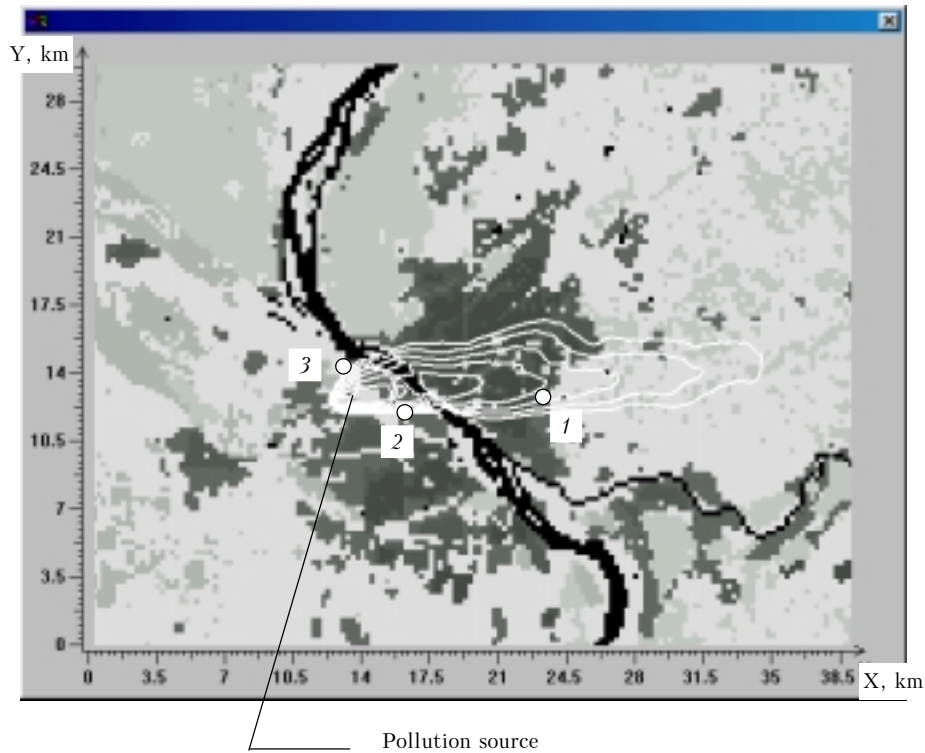


Fig. 1. Map of the area for which the computations were carried out.

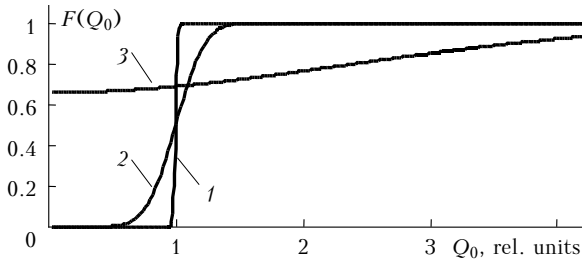


Fig. 2. Distribution function of the emission rates calculated at the points numbered in Fig. 1.

To determine the Eulerian time scale τ , we used the estimate $\tau = 45 z / \bar{U}$ proposed in Ref. 1; here z is the height of the observation point, m; \bar{U} is the mean value of the horizontal component of wind velocity, m/s. We can see that the distributions of the emission rates estimated at the selected points are different in principle. At the first point lying on the lee side, there is almost no scatter in the estimated emission rate. At the second point, the errors in determination of the emission rate become marked. As to the third point, it has no prospects for determination of the source emission rate. The probability to observe zero emission rate at this point exceeds 60%. Similar pattern is also observed when taking into account the measurement errors in concentration.

As an example, Fig. 3 depicts the probability density function for the emission rate estimated at the first point after normalization to the maximum value. Figure 3a corresponds to the model of conditional

variance of a measured result $s_q^2 = \alpha_1^2 J^2$ for $\alpha_1 = 0.2$. Figure 3b corresponds to the conditional variance of a measured result $s_q^2 = \alpha_2^2 J \bar{J}$ for $\alpha_2 = 0.2$.

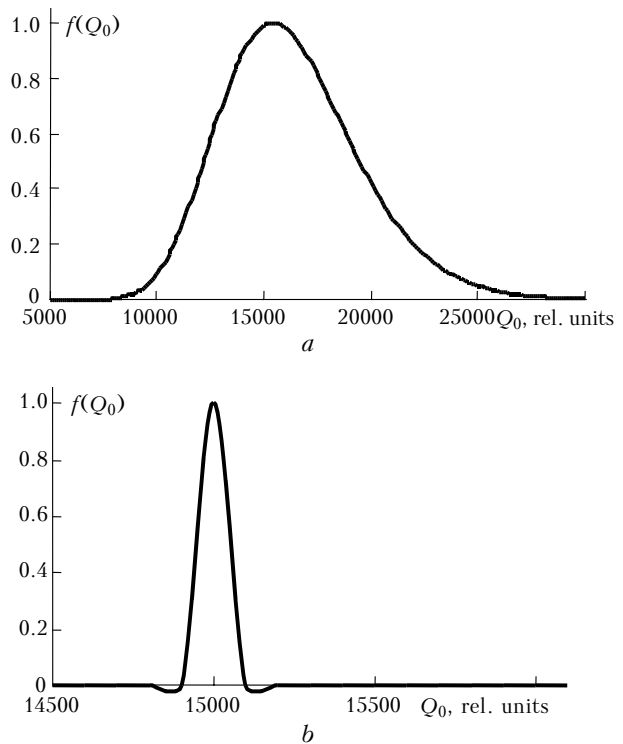


Fig. 3. Probability density function of the estimated source emission rate.

The Table presents standard deviations of the estimated emission rate (18) normalized to the mathematical expectation. We can see that the errors of determination of the source emission rate significantly depend on the peculiarities of the technique used for measurement of the pollutant concentration.

Table

Point	Model $s_q^2 = \alpha_1^2 J^2$	Model $s_q^2 = \alpha_2^2 J \bar{J}$
1	0.21	0.02
2	0.34	0.06
3	0.75	0.16

Thus in this paper we have considered the theoretical basis for accounting for measurement errors of the pollutant concentration in determining the source emission rate through solution of the inverse problem of pollutant diffusion. Practical examples demonstrate the importance of this factor in particular applied problems.

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References

1. A.I. Borodulin, G.M. Maistrenko, and B.M. Chaldin, *Statistical Description of Aerosol Diffusion in the Atmosphere. Method and Applications* (Novosibirsk State University Publishing House, Novosibirsk, 1992), 124 pp.
2. B.M. Desyatkov, S.R. Sarmanaev, and A.I. Borodulin, *Atmos. Oceanic Opt.* **9**, No. 6, 517–520 (1996).
3. B.M. Desyatkov, S.R. Sarmanaev, A.I. Borodulin, S.S. Kotlyarova, and V.V. Selegei, *Atmos. Oceanic Opt.* **12**, No. 2, 130–133 (1999).
4. G.I. Marchuk, *Mathematical Simulation in the Problem of Environment* (Nauka, Moscow, 1982), 320 pp.
5. A.S. Monin and A.M. Yaglom, *Statistical Fluid Mechanics: Mechanics of Turbulence* (MIT Press, Cambridge, Mass., 1971).
6. W. Rodi, in: *Prediction Methods for Turbulent Flows*, ed. by W. Kollmann, (Hemisphere, NY, 1980).