PLANNING AND ANALYZING OBSERVATIONS IN THE PROBLEMS ON ESTIMATION OF THE ZONES OF INFLUENCE AND PARAMETERS OF SOURCES OF THE ATMOSPHERIC POLLUTION

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Based on the K–theory models for turbulent diffusion, Gaussian plume, and approximation equations for the convective conditions, considered are the inverse problems on reconstructing the concentration fields and the parameters of the stationary sources of pollution in the boundary atmospheric layer. We also propose a scheme for making optimal plans of observations. The results of numerical simulations are presented for estimating the source parameters and constructing the optimal plans of observations based on the data of laboratory and field experiments.

When performing under-plume observations aimed at estimating the zone of influence and the parameters of a pollution source under study, one faces the problem on interpretation of observational results and optimal arrangement of the observational network. To solve this problem, it is worthwhile to use additional information on the meteorological conditions, pollutant spread processes, source characteristics, capabilities of the measurement network, etc.

This paper concerns the problems of reconstructing the field of the near-ground concentration of pollutants and the parameters of stationary sources from the data of laboratory and field experiments. To describe the process of a pollutant spread in the near-ground and boundary layers of the atmosphere, we use the models of K-theory of the gradient transport, the Gaussian statistical model, and the empirical approximation equations for the experimental data. The wind velocity, the turbulent exchange coefficients, and the diffusion parameters are either preset on the basis of corresponding parametrizations or computed using models of the boundary atmospheric layer.

The main parameters to be estimated are the position of maximum near-ground concentration and its level there, the coefficient of plume broadening in the direction normal to the wind, the emission power, and the effective height of a source. In the case of a heavy pollutant, the parameters taking account of the joint effects of particle sedimentation and turbulent mixing should be estimated too.

The estimation models proposed were tested on the data of laboratory observations as well as field experiments near heat power stations and aerosol sources with controllable parameters. The proper choice of the arrangement of sampling points is shown to be efficient as regards the accuracy of the parameters reconstruction.

1. PLANNING OF OBSERVATIONS

By the plan of an experiment we understand the set $\varepsilon_N = \{x_i, p_i\}_{i=1}^N$, where p_i is the number of measurements at the point $\mathbf{x}_i$, N is the total number of observations. The optimal plan ε_N^* is sought by solving the extremum problem

$$|D(\varepsilon_N^*, \hat{\theta}_N)| = \inf_{\varepsilon_N} |D(\varepsilon_N, \hat{\theta}_N)|.$$

Here $D = M^{-1}$, M is the Fisher information matrix; D is the matrix of the estimate variances:

$$M(\varepsilon, \theta) = F\,F^T,$$

where

$$F = ||\,\mathbf{f}(\mathbf{x}_1, \theta), \dots, \mathbf{f}(\mathbf{x}_n, \theta)||, \;\; \mathbf{f}^T = \left|\left| \frac{\partial q}{\partial \theta_1}, \dots, \frac{\partial q}{\partial \theta_m} \right|\right|;$$

q is the pollutant concentration, θ is the vector of unknown parameters. Generally speaking, since the regression dependence $q(\boldsymbol{x}, \theta)$ is nonlinear with respect to θ, the optimal plan is sought using the following iteration procedure of sequential analysis and planning of observations.[1]

1) Let the experiment be conducted based on a nondegenerate plan ε_N (i.e. $|M(\varepsilon_N, \hat{\theta}_N)| \neq 0$).

2) Find the estimate $\hat{\theta}$ by the least-square method following this plan.

3) Find the point

$$\mathbf{x}_{N+1} = \arg \sup_{\mathbf{x} \in \Omega} d(\mathbf{x}, \varepsilon, \hat{\theta}_N),$$

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where $d(\mathbf{x}, \varepsilon_N, \hat{\theta}_N) = \mathbf{f}^T(\mathbf{x}, \theta)\, M^{-1}(\varepsilon_N, \theta)\, \mathbf{f}(\mathbf{x}, \theta)\Big|_{\theta=\hat{\theta}_N}$ is the variance of the concentration field; Ω is the domain of planning.

4) Perform an additional observation at the point $\boldsymbol{x}_{N+1}$. Then repeat the steps 1 to 3.

2. RECONSTRUCTION OF THE NEAR-GROUND CONCENTRATION FIELD PRODUCED BY A GAS–AEROSOL SOURCE

Let the process of a pollutant dispersal from a stationary source with a height H be described by the equation

$$u(z)\,\frac{\partial q}{\partial x} - w\,\frac{\partial q}{\partial z} = \frac{\partial}{\partial z}\,k(z)\,\frac{\partial q}{\partial z} + \frac{\partial}{\partial y}\,v(z)\,\frac{\partial q}{\partial y} \qquad (1)$$

with the boundary conditions

$$k\,\frac{\partial q}{\partial z}\Big|_{z=0} = 0,\quad q\,\Big|_{|\mathbf{x}|\to\infty} \to 0,\quad uq\,\Big|_{x=0} =$$

$$= Q\,\delta(y)\,\delta(z-H), \qquad (2)$$

where $\boldsymbol{x} = (x, y, z)$, with the x axis being directed along the wind and the z axis looking vertically upward; $u(z)$ is the wind velocity, and $\delta(z)$ is the delta function.

Approximating the wind profiles and the coefficients of turbulent exchange by power-law functions of height, from Eqs (1) and (2) we derive the expression for the near-ground concentration in the form of nonlinear regression function

$$q(\mathbf{x}, \theta) = \frac{\theta_1}{x^{3/2}}\,\exp\left(-\frac{\theta_2}{x} - \frac{\theta_3\, y^2}{x}\right) \times$$

$$\times \sum_{i=1}^{K} p_i\,\frac{\theta_2^{\theta_4 w_i}}{\Gamma\,(1 + w_i\,\theta_4)\; x^{\theta_4 w_i}}, \qquad (3)$$

where $\theta = (\theta_1, \theta_2, \theta_3, \theta_4)^T$ is the vector of the parameters sought. As an additional information, we use here the measurement data on the near-ground concentration

$$r_k = q(\mathbf{x}_k, \theta) + \xi_k, \quad k = \overline{1, N}\,. \qquad (4)$$

The vector of the parameters sought, θ, and the regression function (3) can be found from the condition of the functional minimum

$$I_N(\theta) = \sum_{k=1}^{N} \sigma_k^{-2}\,(r_k - q(\mathbf{x}_k, \theta))^2. \qquad (5)$$

Figure 1 shows the results of reconstruction of the axial near-ground concentration of a sedimenting pollutant from a point source at a height H = 100 m for three versions of observational plans using the models (3)–(5). As follows from this figure, the highest accuracy of reconstruction is reached when using the optimal plan of observations.[2]

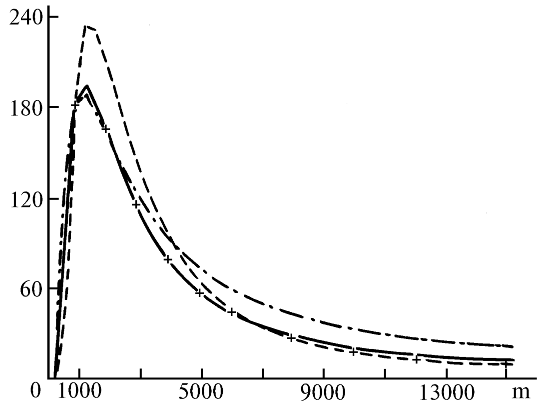

FIG. 1. The axial concentration (cm$^{-5/2}$ s) *of a monodisperse pollutant for* w = 20 cm/s *reconstructed using the locally D – optimal plan (solid line), the uniform plan (dashed line), the two–point plan (dot-and-dash line) and calculated by the model (1)–(2) (crosses).*

3. THE INVERSE PROBLEM OF ESTIMATING THE SOURCE PARAMETERS

Based on the model (1) – (2), the Gaussian model of a plume and the data of near-ground concentration observations, by solving the inverse problem, the emission power Q and the effective height H of a source are determined.[3] As observational data we use the experimental data on the state of the atmospheric boundary layer and the SO_2 concentration in the vicinity of the heat power station in Diccerson (Canada).[4] Table I gives the results on Q and H estimation.

TABLE I. The reduced emission power Q and the effective height H of a source estimated by the mixed model.

Serial number of a case	Points of the plan x, m	q_{cal}/q_{exp}	Estimates Q	Estimates H, m	H_{exp}, m
1	2111	1.3			
	8129	1.7	0.6	120	145
2	1724	1.1			
	5660	1.2	0.8	110	130
3	5660	0.6			
	14600	1.1	0.9	190	135
4	3106	1.1			
	8670	1.9	0.5	95	124
5	3106	1.1			
	5293	0.9	1.0	130	125
6	3106	1.1			
	5600	1.2	0.8	120	124

In the case of a convective boundary layer of the atmosphere, the Briggs approximation formula[5] is used to describe the near-ground concentration:

$$q(X, Z_h, Q) = Q\,\Psi(X, Z_h)$$

$$\Psi(X, Z_h) = \frac{0.9\,(X/Z_h)^{9/2}}{[1 + 0.4\,(X/Z_h^{5/6})^{9/2}]^{4/3}} +$$

$$+ [1 + 3\,Z_h^{1/2}\,X^{-3/2} + 50\,X^{-9/2}]^{-1}, \qquad (6)$$

which describes quite adequately the data of laboratory experiments.[6] In Eq. (6) q is the near-ground concentration of a pollutant, h and $Z_h = h/z_i$ is the true and relative heights of the source, z_i is the height of the mixing layer, Q is the emission power of a linear source.

Table II gives the results of Q and Z_h reconstruction using the regression dependence (6) on a set of plans formed by all possible pairs of observation points X_i, $i=\overline{1,12}$. It follows from the table that with the relatively close correspondence between the measured concentrations and those calculated by Eq. (6), the plans with smaller values of the determinant of the variance matrix yield better estimates.

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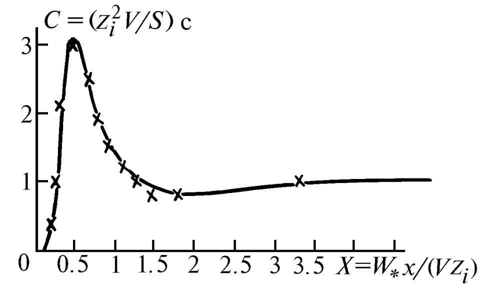

FIG. 2. The axial near-ground concentration produced by a source with height Z_h = 0.24 calculated by the Briggs formula (solid line) and the Willis and Deardorff laboratory results (crosses).

TABLE II. Distribution of the relative error of estimation of the parameters $\hat{Z}_h$ and $\hat{Q}$ *on the set of plans* ε_{ij} *at* Z_h = 0.24.

	x2										
x1	a2	a3	a4	a5	a6	a7	a8	a9	a10	a11	a12
a1	146/Δ	94/Δ	2/•	5/•	5/•	8/•	7/•	8/•	13/•	2/•	7/•
a2		76/•	3/•	6/•	5/•	9/•	6/•	7/•	13/•	2/•	8/•
a3			6/•	7/•	5/•	7/•	5/•	6/•	11/•	3/•	7/•
a4				10/•	4/•	7/•	4/•	5/•	107/•	2/•	13/•
a5					76/Δ	62/Δ	51/Δ	42/Δ	32/Δ	16/Δ	8/Δ
a6						56/Δ	5/Δ	34/Δ	22/Δ	33/Δ	96/Δ
a7							45/Δ	26/Δ	8/Δ	48/Δ	153/Δ
a8								15/Δ	13/Δ	113/Δ	226/Δ
a9									31/Δ	170/Δ	299/Δ
a10										290/Δ	46/Δ
a11											27/Δ

Note. Numerator: $\max\left\{\frac{|Z_h - \hat{Z}_h|}{Z_h}, \frac{|Q - \hat{Q}|}{Q}\right\}$ 100%, denominator: • for $|D(\varepsilon_{ij})| \le 0.2$; Δ for $|D(\varepsilon_{ij})| > 0.2$.

Shown in Fig. 3 are the results of numerical simulation of the optimal measurement plans according to the procedure given in Section 1 depending on the source height Z_h sought, under the condition when the domain of planning falls within the interval [0.6; 4]. It is seen from the figure that up to a certain height Z_h the interval ends are more informative. A sharp change in the points position in the plan occurs when $X_{\max}(Z_h) > 0.6$. Here $X_{\max}(Z_h)$ is the point of the maximal near-ground concentration.

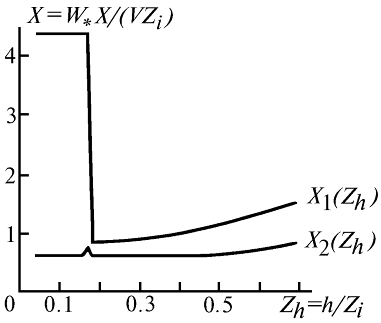

FIG. 3. Locally D–optimal plans of observations in the inverse problem of estimating Q and Z_h parameters for the convective planetary boundary layer.

4. ESTIMATION OF THE EMISSION TOTAL OUTCOME

Sometimes it is very important to have an estimate of the total outcome of emissions coming from a territory.

Let in a 3D limited area Ω there are M pollution sources with the power θ_m, $m = \overline{1,M}$. The process of a pollution dispersion spread from each source is described by the corresponding model (1) – (2). Then, having available the data of concentration measurements in Ω, one can formulate the following problems on estimating the minimal and maximal total emission outcome possible under these conditions:

Find the vector $\boldsymbol{\theta} = (\theta_1, \ldots, \theta_M)^T$ *such that*

$$R(\boldsymbol{\theta}) = \sum_{m=1}^{M} \theta_m \to \max_{\boldsymbol{\theta}\in D} \; (\min_{\boldsymbol{\theta}\in D}),$$

under the limitations

$$\sum_{m=1}^{M} a_{nm}\, \theta_m \le r_n \; (\ge r_n), \quad n = \overline{1, N}\ ;$$

$$D = \{\boldsymbol{\theta} : 0 \le A_m \le \theta_m \le B_m, \;\; m = \overline{1, M}\ \}.$$

Here a_{nm} is the concentration produced by a single emission from the mth source at the point X_n, r_n is the concentration measured at the point X_n, A_m and B_m are the lower and the upper boundaries of admissible values of the mth source emission power.

Using as an example the area of the Barnaul chemical fiber plant, numerical experiments were performed aimed at estimation of the upper and lower boundaries of the total H_2S emission from 17 sources based on the data of routine observations depending on the index of stability μ_0 of the boundary atmospheric layer.[7]

The results of numerical simulation shown in Fig. 4 demonstrate a close agreement of the estimates obtained with the total emission outcome sought being equal to 95 g/s under unstable atmospheric stratification.

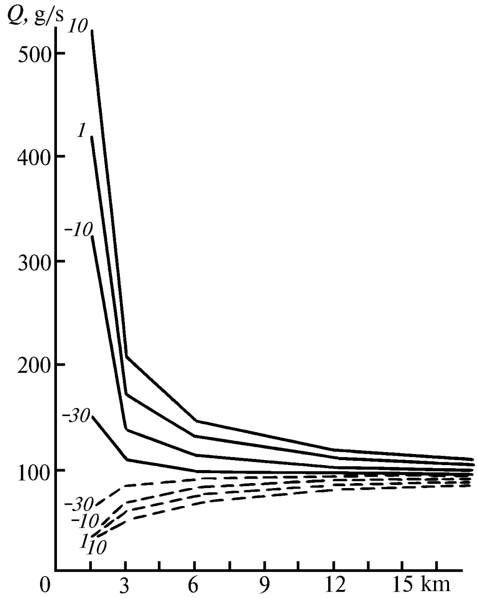

FIG. 4. The estimates of the upper, Q_{max} (solid line), and lower, Q_{min} (dashed line), boundaries of the total emission at μ_0 = 10, 1, –10, –30 *against the distance x (for the near-ground layer).*

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