PROBLEM ON ESTIMATING THE TOTAL STRENGTH OF ATMOSPHERIC POLLUTION SOURCES

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This paper considers optimization models for estimating the total strength of industrial emissions of pollution sources based on concentration measurements at the ground level or at a fixed altitude. The upper and lower limits of emission strength for individual sources, regions of characteristic pollution, typical meteorological conditions, and peculiarities of an observation system are the necessary additional data for solving inverse problems. Numerical experiments on estimation of the upper and lower limits of the hydrogen sulfide emission strength for different positions of the observation system under various meteorological conditions have been carried out by the example of an industrial area of the Barnaul Integrated Chemical Fiber Plant. Analysis of the results of numerical simulation has shown the satisfactory agreement of estimates with a given total emission strength under conditions of unstable atmospheric stratification.

When mathematically simulating the processes of pollutant transport in the atmosphere, of fundamental importance are the inverse problems associated with the estimate of the parameters of pollution sources. This line of investigation is represented by the theoretical and applied investigations devoted to the justification of the statement of problems and numerical methods for their solution.[1–3] The use of the mathematical model of pollutant transport and *a priori* information about the parameters of sources, structure, and precision of observations makes it possible to solve the problem of estimating the emission strength from a number of sources.

The paper considers optimization models of estimating the total strength of pollutant emission from the data on ground and elevated concentration. As a goal function, the total strength of emission sources is used. Models of the pollutant transport and of the atmospheric boundary layer (ABL) are believed to be the basic limitations in the estimation problem. Additional information in solving the inverse problems is the following: the upper and lower limits of the emission strength for individual sources, regions of typical pollution, typical meteorological conditions, and peculiarities of an observation system.

Numerical experiments on estimating the upper and lower limits of the total hydrogen sulfide emission strength for different observation systems under various meteorological conditions have been carried out by the example of an industrial area of the Barnaul Integrated Chemical Fiber Plant (ICFP). Analysis of the results of numerical simulation has shown satisfactory agreement of the estimates with a given total strength under conditions of unstable stratification of the atmosphere. Histograms of the estimates of the upper and lower limits of total emission strength were constructed depending on the distance to the industrial area.

1. MODELS OF THE PLANETARY BOUNDARY LAYER OF THE ATMOSPHERE AND POLLUTANT TRANSPORT

For calculation of the vertical profiles of the mean wind velocity and the coefficient of vertical turbulent exchange, which are the input parameters for a model of atmospheric diffusion, we use the model of the temperature-stratified atmospheric boundary layer proposed in Ref. 4.

The model describing stationary and horizontally-homogeneous flows in the boundary layer contains a set of equations of hydrodynamics of the turbulent atmosphere in the form

$$\frac{\mathrm{d}}{\mathrm{d}z}\, k\, \frac{\mathrm{d}u}{\mathrm{d}z} + f(v - v_g) = 0,$$

$$\frac{\mathrm{d}}{\mathrm{d}z}\, k\, \frac{\mathrm{d}v}{\mathrm{d}z} - f(u - u_g) = 0, \qquad (1)$$

$$k\left[\left(\frac{\mathrm{d}u}{\mathrm{d}z}\right)^2 + \left(\frac{\mathrm{d}v}{\mathrm{d}z}\right)^2\right] + \frac{g}{\overline{T}}\,\frac{P(z)}{c_p\,\rho} + \alpha_b\,\frac{\mathrm{d}}{\mathrm{d}z}\, k\,\frac{\mathrm{d}b}{\mathrm{d}z} - \varepsilon = 0,$$

$$k\left[\left(\frac{\mathrm{d}u}{\mathrm{d}z}\right)^2 + \left(\frac{\mathrm{d}v}{\mathrm{d}z}\right)^2\right] + \alpha_1\,\frac{g}{\overline{T}}\,\frac{P(z)}{c_p\,\rho} + \alpha_2\,\frac{b}{\varepsilon}\,\frac{\mathrm{d}}{\mathrm{d}z}\, k\,\frac{\mathrm{d}\varepsilon}{\mathrm{d}z} - \alpha_3\varepsilon = 0, \qquad (2)$$

$$k = \alpha_\varepsilon\,\frac{b^2}{\varepsilon},$$

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where α_b, α_1, α_2, α_3, and α_ε are the empirical constants; $P(z)$ is the turbulent heat influx; T is the mean temperature within the limits of the atmospheric boundary layer; b is the turbulent kinetic energy; ε is the rate of the turbulent energy dissipation in heat.

The boundary conditions are

$$u = v = 0, \quad b = b_0, \quad \varepsilon = \varepsilon_0 \quad \text{at } z = z_0.$$

At the upper boundary ($z = h$) they are

$$u \to u_g,\ v \to v_g,\ b \to 0,\ \varepsilon \to 0.$$

Based on an asymptotic formula for the gradient of the potential temperature in the atmospheric boundary layer[5] (ABL), the turbulent heat flux $P(z)$ is calculated as follows:

$$P(z) = k\left[\frac{P_0}{\varkappa\, v_*\, z} - \rho\, c_p(\gamma_a - \gamma_h)\left(\frac{z}{h}\right)^m\right], \tag{3}$$

where $\gamma_h = 0.6°\text{q}/100$ m is the temperature gradient in the free atmosphere, v_* is the dynamic velocity scale; P_0 is the surface heat flux, h is the atmospheric boundary layer height, and κ is von Karman's constant.

Proceeding to dimensionless variables

$$u_n = \varkappa\, u/v_*, \quad v_n = \varkappa\, v/v_*, \quad \eta_n = \eta/v_*^2, \quad \sigma_n = \sigma/v_*^2,$$

$$z_n = z/L_1, \quad L_1 = \varkappa\, v_*/f, \quad \theta = \theta/\theta_*,$$

$$\theta_* = -\,P_0/(c_p\, \rho\, v_*),$$

$$k_n = k/(\varkappa v_* L_1),\ b_n = b/(\alpha_\varepsilon^{-1/2} v_*^2),\ \varepsilon_n = \varepsilon/(v_*^3/\varkappa\, L_1),$$

$$\mu = \mu_0\, k_n \frac{d\theta_n}{dz_n} = \mu_0\left(k\,\frac{d\theta}{dz}\right)/(P_0/(c_p\,\rho)),$$

$$z_{0n} = z_0/L_1,\ z_{0n} = (\varkappa^2\,\chi\, Ro)^{-1}$$

makes it possible to write the initial equations as function of only one parameter $\mu_0 = L_1/L$, where $L = -\,v_*^3/(\varkappa\,(g/\overline{T}\,)\,P_0/(c_p\,\rho))$ is the Monin–Obukhov length, $\chi = v_*/\varkappa c_g$ is the geostrophic friction coefficient, and $Ro = c_g/(fz_0)$ is the Rossby number.

In the dimensionless form, a closed set of ABL equations (1)–(2) is:

$$\frac{d^2\eta_n}{dz_n^2} + \frac{\sigma_n}{k_n} = 0,$$

$$\frac{d^2\sigma_n}{dz_n^2} - \frac{\eta_n}{k_n} = 0, \tag{4}$$

$$\frac{\eta_n^2 + \sigma_n^2}{k_n} - \mu + \beta_1 \frac{d}{dz_n}\, k_n \frac{db_n}{dz_n} - \varepsilon_n = 0, \tag{5}$$

$$\frac{\eta_n^2 + \sigma_n^2}{k_n} - A_3\,\mu + A_1 \frac{k_n}{b_n}\frac{d}{dz_n}\, k_n \frac{d\varepsilon_n}{dz_n} - A_2\,\varepsilon_n = 0, \tag{6}$$

$$k_n = b_n^2/\varepsilon_n,$$

$$\mu = \frac{k_n}{z_n}\left(\mu_0 + \frac{\varkappa^4\,(\gamma_a - \gamma_h)\,g\,z_n^2}{f^2\,\overline{T}\,h}\right), \tag{7}$$

$$\mu_0 = -\,\frac{\varkappa^2\,g\,P_0}{f\,\rho c_p\,\overline{T}\,v_*^2}.$$

Boundary conditions are

$$\eta_n = 1, \quad \sigma_n = 0, \quad b_n = 1, \quad \varepsilon_n = \varkappa^2\,\chi\,Ro, \quad u_n = v_n = 0$$

$$\text{at } z_n = (\varkappa^2\,\chi\,Ro)^{-1}, \tag{8}$$

$$\eta_n \to 0, \quad \sigma_n \to 0, \quad b_n \to 0, \quad \varepsilon \to 0 \quad \text{when } z_n \to \infty.$$

As optimal values of the constants β_1, A_1, A_2, and A_3, the following values were selected: $\beta_1 = 0.41$, $A_1 = 0.31$, $A_2 = 1.31$, and $A_3 = 0.70$, obtained in Ref. 4 based on the analysis of the effect of numerical constants on the ABL characteristics.

The solution of the set of equations (4)–(6) is constructed by its separation into subsystem (4) and equations (5) and (6). The set of algebraic equations obtained as a result of the finite-difference approximation of equations of motion on a nonuniform grid is solved by the matrix pass technique. As a result, we calculate the vertical profile of the components of the tangent stress vector η_n and σ_n. The numerical solution of Eqs. (5) and (6) by the pass technique enables one to determine b_n and ε_n.

To describe the spread of pollutant from a continuous source located in three-dimensional bounded region $\Omega = \Gamma\times[0, h]$, we use the stationary semiempirical equation of turbulent diffusion[6]:

$$Lq \equiv \mathbf{u}\,\nabla q + \alpha q - \frac{\partial}{\partial z}\,k_z\,\frac{\partial q}{\partial z} - \operatorname{div}_s \nu\,\nabla_s q = \theta\varphi(\mathbf{x}) \tag{9}$$

with the boundary conditions

$$k_z\,\frac{\partial q}{\partial z} + \beta q\,\Big|_{z=z_0} = 0,$$

$$\frac{\partial q}{\partial z}\Big|_{z=h} = 0,$$

$$q\,|_\Gamma = F, \quad q\,|_{\mathbf{x}=0} = q_0(y, z), \tag{10}$$

where $q(\mathbf{x})$ is the pollutant concentration at the point $\mathbf{x} = (x, y, z)$; $\mathbf{u}(x)$ is the wind velocity; ν and k_z are the coefficients of horizontal and vertical turbulent exchange; α, β, and q_0 are the known functions of coordinates; F is the value of concentration at the lateral boundary Γ of the region Ω; div_s and ∇_s are the operators of divergence and gradient in the horizontal direction; $\varphi(\mathbf{x})$ is the function describing the position of the source in the region Ω; θ is the source strength.

2. FORMULATION OF THE PROBLEM OF ESTIMATION

We assume that M sources are in the region Ω. Then the process of pollutant transport from the sources is described by the equation

$$Lq = \sum_{m=1}^{M} \theta_m \varphi_m(\mathbf{x}) \qquad (11)$$

with boundary conditions (10). Here, $q(\mathbf{x})$ is the total concentration at a point $\mathbf{x}$; $\varphi_m(\mathbf{x})$ is the function specifying the position of the mth source in the region Ω, and θ_m is its strength.

In view of the principle of superposition, the solution of problem (11)–(10) can be determined as follows:

$$q(\mathbf{x}, \boldsymbol{\theta}) = \Phi(\mathbf{x}) + \sum_{m=1}^{M} \theta_m \psi_m(\mathbf{x}), \qquad (12)$$

where ψ_m is the solution for the mth source of unit strength with zero boundary conditions (10) and $\Phi(\mathbf{x})$ is the background concentration value.

For determining the unknown coefficients θ_m, $m = \overline{1, M}$, there is a need for information about the concentration fields inside the region Ω and at its boundary. We assume that the concentration measurements are carried out at points $\mathbf{x}_1,\ldots,\mathbf{x}_N \in \Omega$

$$y_n = q(\mathbf{x}_n, \boldsymbol{\theta}) + \xi_n,$$
$$E[\xi_n] = 0, \;\; E[\xi_n \xi_{n'}] = \delta_{nn'} \sigma_n^2, \;\; n, n' = \overline{1, N}, \qquad (13)$$

where ξ_n is the measurement error.

If the standard deviation of calculated and measured values of the pollutant concentration is considered as a goal function, under definite conditions one can obtain the estimate of source strengths[3,7]

$$\hat{\boldsymbol{\theta}} = C^{-1} Y, \qquad (14)$$

where $\boldsymbol{\theta}^T = (\theta_1,\ldots,\theta_M)$, C is the Fisher information matrix, Y is the vector of dimension M,

$$C = \sum_{i=1}^{N} \sigma_i^{-2} \psi(\mathbf{x}_i) \psi^T(\mathbf{x}_i),$$

$$Y = \sum_{i=1}^{N} \sigma_i^{-2} \psi(\mathbf{x}_i) [y_n - \Phi(\mathbf{x})],$$

$\boldsymbol{\Psi}^T = (\psi_1,\ldots,\psi_M)$. The estimate (14) is valid if the matrix C is nondegenerate. This condition is satisfied when the number of observation points N is no less than the number of sources M, but this is not always the case. In addition, there is a need for optimal arrangement of the observation system to obtain stable estimates of the vector $\boldsymbol{\theta}$.

In some cases, Eq. (14) is invalid, for example, when $N < M$. In this connection, of considerable interest is the estimate of the lower and upper limits of the total emission strength of industrial pollutant from the data of concentration measurements in the atmosphere.

Let us consider the following problem of determination of the lower limit of the total emission strength.

Problem 1. To find the vector $\boldsymbol{\theta} = (\theta_1,\ldots,\theta_M)^T$ such that

$$R(\boldsymbol{\theta}) = \sum_{m=1}^{M} \theta_m \to \max_{\boldsymbol{\theta}\in D} \qquad (15)$$

under constraints

$$q(\mathbf{x}_n, \boldsymbol{\theta}) \le y_n, \quad n = \overline{1, N}.$$

Here, $D = \{\theta_m : 0 \le A_m \le \theta_m \le B_m, \; m = \overline{1, M}\}$, A_m and B_m are the limiting permissible values of emission strength for the mth source. The problem of estimating the upper limit is formulated similarly.

Problem 2. To determine the vector $\boldsymbol{\theta} = (\theta_1,\ldots,\theta_M)^T$ such that

$$J(\boldsymbol{\theta}) = \sum_{m=1}^{M} \theta_m \to \min_{\boldsymbol{\theta}\in D} \qquad (16)$$

under constraints

$$q(\mathbf{x}_n, \boldsymbol{\theta}) \ge y_n, \quad n = \overline{1, N}.$$

Taking into account Eq. (12), problems 1 and 2 reduce to those of the linear programing that are numerically solved with the use of standard programs.

3. NUMERICAL EXPERIMENTS

Calculations of the total emission strength from a number of industrial sources were made with the use of the model of pollutant transport with the solution in the form of total concentration

$$\bar{C}_y = \int_{-\infty}^{\infty} q(x, y, z)\, dy. \qquad (17)$$

The use of Eq. (17) enables us to solve Eqs. (15) and (16) without consideration of transverse diffusion. Such a simplification results in a simpler structure of observations.

The industrial area chosen for numerical experiments was the territory of the Barnaul Integrated Chemical Fiber Plant where 17 sources of hydrogen-sulfur-containing emission were located. Figure 1 shows the scheme of the industrial area with the sources of hydrogen-sulfur-containing emissions, on a 1:250 m scale in the principal coordinate system. The data on the parameters of the sources were taken from the Ecological Certificate of this Plant, according to which the heights of sources varied from 20 to 125 m. The mean wind was in the southwest direction.

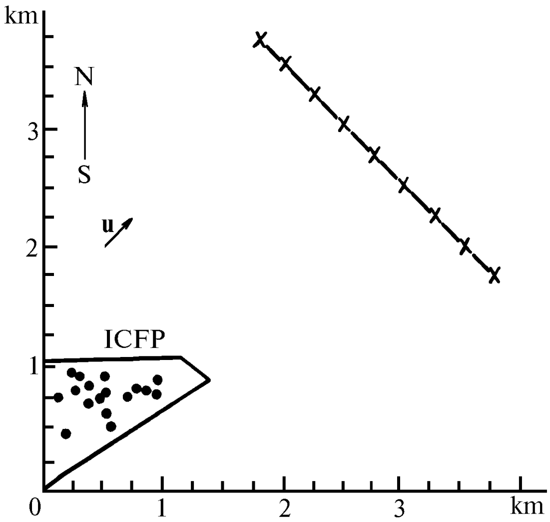

FIG. 1. Scheme of the Integrated Chemical Fiber Plant (ICFP), pollution sources, and route observations.

The problem on the total emission strength was solved for different turbulent modes of the ABL characterized by the dimensionless Monin–Kazanskii parameter μ_0 varying in the range from 10 to −30. With these values, the vertical profiles of the mean wind velocity and the coefficient of turbulent diffusion were calculated for the stationary ABL. The problem was solved for model values of the total concentration produced by a number of sources. The observation routes were chosen in the direction transverse to the wind at distances from the coordinate origin 1.5, 3, 6, 12, 18 km. The further increase of the distance from the sources makes no sense, because according to Refs. 8 and 9, when the condition

$$2\sigma_z(x) + (h + \Delta h) > z_i$$

is satisfied, which is usually the case at large distances, the total concentration becomes weakly dependent on the coordinate x:

$$\bar{C}_y \simeq Q/(u\, z_i). \tag{18}$$

Here, h is the geometric height of the source, Δh is the height due to thermal and dynamic rise of a plume, z_i is the mixing layer height, and $\sigma_z^2(x)$ is the variance of vertical diffusion of pollutant.

The results of numerical experiments are shown in Figs. 2 and 3. From our calculations, it follows that as the distance from the industrial area increases, the estimates Q_{max} and Q_{min} approach from above and below the same value, namely, the given total strength (95 g/s) of the sources under study. Analysis of the behavior of estimates of total emission strength enables us to note the following peculiarity of the pollutant diffusion from the number of sources based on model (9)–(10): in the vicinity of the industrial area at distances up to 1.5 km for the ground-based observations, the values of Q_{max} are overestimated; for an observation height of about 200 m, such a tendency remains up to 6 km. The overestimated values of Q_{max} and Q_{min} are observed in the case of the stably stratified ABL as compared with the convective one. This is due to the decrease of the vertical turbulent exchange under stable conditions.

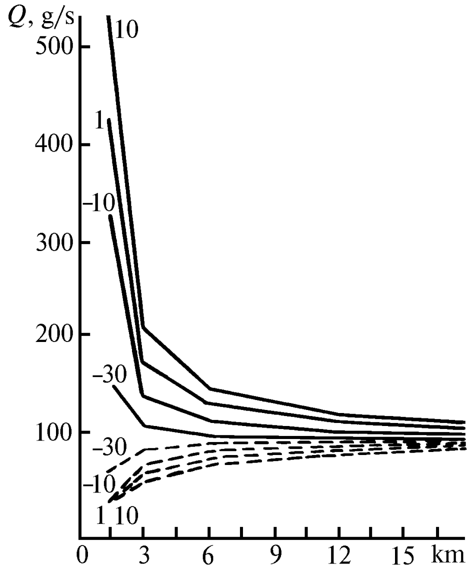

FIG. 2. The behavior of the estimates of the upper (Q_{max}) and lower (Q_{min}) limits of the total emission strength at μ_0 = 10, 1, −10, and −30, *as functions of the distance x (for the atmospheric ground level): solid curve denotes* Q_{max} *and dashed curve denotes* Q_{min}.

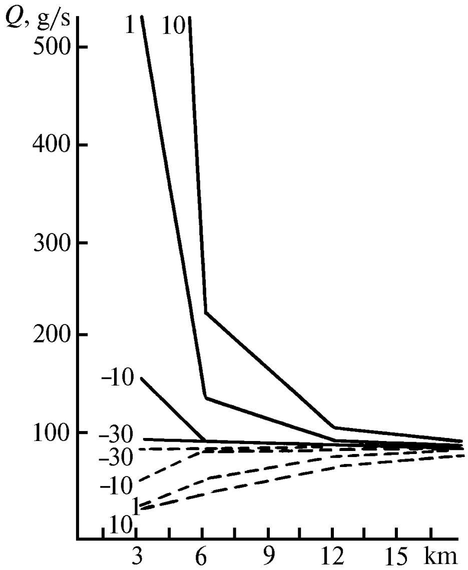

FIG. 3. The behavior of the estimates Q_{max} *and* Q_{min} *at* μ_0 = 10, 1, −10, and −30, *as functions of the distance x (for a height of about* 200 m*): solid line denotes* Q_{max} *and dashed line denotes* Q_{min}.

Our numerical experiments enable us to draw the following conclusions:

– for the models of the stationary ABL and pollutant transport we have obtained the numerical solutions of optimization problems for the upper and lower limits of the total emission strength from a number of sources;

– the character of the behavior of estimates of the upper and lower limits, as the distance from the industrial area increases, is representative of the qualitative behavior of solutions to pollutant transport equations under conditions of uniform vertical distribution of the total concentration;

– the quality of estimates points to the validity of the given statements of optimization problems for calculation of the limits of total emission strength;

– under considered conditions of applicability of the above-indicated models of the ABL and the pollutant transport, the agreement between estimates and the given total strength is quite satisfactory for unstable stratification.

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