

OPTIMIZATION OF MODELS FOR CONTROL AND MONITORING OF AEROSOL SOURCES

V.F. Raputa and A.I. Krylova

*Computing Center,
Siberian Branch of the Russian Academy of Sciences, Novosibirsk
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In this paper we consider the problems on optimal regulation of aerosol sources in the ground atmospheric layer, estimation of sources parameters, and optimization of the observational network. Analysis is made based on semiempirical equation of turbulent diffusion. To illustrate the approach used, we give examples of solutions of the inverse problems on estimating capacity and location of sources. Examples of optimal distribution of the observational points taking into account meteorological situation and configuration of aerosol sources are given in this paper. We also present some results of numerical experiments on modeling optimal modes of treatment of agricultural crops with aerosols produced by a generator capable to regulate disperse composition of aerosol.

Investigations of spreading and accumulation of pollutants, peculiarities of their local circulations and spatiotemporal distributions are the basis for an objective estimate of the state of the air basin and tendencies in air pollution variations. Mathematical simulation plays a significant role in these investigations. Along with the conventional statements of the problems it allows one to study new problems arising in the monitoring of air pollution, the regulation of sources, their optimum location, etc.

The problems of optimum control of aerosol sources, the estimation of zones of their impact from observational data and their parameters are considered. The problem on optimization of observational system is considered separately.

Let the point source of pollution be in a three-dimensional domain $\Omega = \omega \times [0, H]$. The location and the capacity of this source are described by the quantities $\mathbf{X} = (X, Y, Z) \in \Omega$ and Q , respectively. The following model is used to describe the transport of pollution^{1,2}:

$$\frac{\partial q}{\partial t} + \mathbf{u} \nabla q + pq - \tilde{\Delta} q = f_1(\mathbf{x}, t) + Q \delta(\mathbf{x} - \mathbf{X}) \gamma(t); \quad (1)$$

$$\left(v \frac{\partial q}{\partial z} + \beta q \right) \Big|_{z=0} = f_2, \quad v \frac{\partial q}{\partial z} \Big|_{z=H} = h_1; \quad (2)$$

$$q \Big|_S = h_2, \quad q \Big|_{t=0} = q_0(\mathbf{x}). \quad (3)$$

Here \mathbf{u} is the vector of wind velocity with the components u , v , and w ; p is the function determining the rate of change in concentration $q(\mathbf{x}, t)$ due to chemical reactions; $\tilde{\Delta} = \frac{\partial}{\partial z} v \frac{\partial}{\partial z} + \text{div}_S \mu \text{grad}_S$ is the operator describing the turbulent exchange in vertical and horizontal directions; S is the lateral boundary of the domain Ω ; f_1 , f_2 , h_1 , h_2 , and q_0 are the functions characterizing the location and the capacity of known sources inside the domain $\Omega_T = \Omega \times [0, T]$ and at its boundary; $\gamma(t) = 0$ at $t \leq t_0$ and $\gamma(t) = 1$ at $t > t_0 > 0$ (δ is delta function; γ is the parameter characterizing the time of source operation; v and μ are the coefficients of turbulent exchange in vertical and horizontal directions).

1. INVERSE PROBLEMS OF POLLUTION DISPERSION. PLANNING OF OBSERVATIONS

A. Estimation of the source strength

Let us assume that the right-hand part of Eq. (1) has the form

$$f(\mathbf{x}, t) = \sum_{m=1}^M \theta_m f_m(\mathbf{x}, t), \quad (4)$$

where $f_m(\mathbf{x}, t)$ are the functions describing the source location and the regime of its operation in time, θ_m is the source capacity, $m = \overline{1, M}$.

Then, by virtue of the superposition principle, a solution of the problem (1)–(3) can be represented as

$$q(\mathbf{x}, t, \theta) = \Phi(\mathbf{x}, t) + \sum_{m=1}^M \theta_m q_m(\mathbf{x}, t), \quad (5)$$

where $q_m(\mathbf{x}, t)$ is the fundamental solution corresponding to the m th source, and $\Phi(\mathbf{x}, t)$ is the solution of Eq. (1) with zero right-hand part and boundary conditions (2) and (3).

Let us assume that measurements are performed in the points $\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_N \in \Omega$, then

$$y_n(t) = q(\mathbf{x}_n, t, \theta) + \varepsilon_n, \quad 0 \leq t \leq \tau,$$

$$E[\varepsilon_n] = 0, \quad E[\varepsilon_n \varepsilon_n] = \delta_{nn'} \sigma_n^2, \quad n \leq N. \quad (6)$$

Here E is the operation of mathematical expectation, $\delta_{nn'}$ is the Kroneker symbol, and τ is the total period of observations.

Assuming that the goal function is the rms deviation of computed and measured concentrations of a pollutant, an estimate of the source capacity³ is obtained in an explicit form

$$\hat{\theta} = C^{-1} \mathbf{Y}, \quad (7)$$

where C is the informational Fisher matrix,

$$Y = \sum_{i=1}^n P_i \int_0^s q(x_i, t) [y_i(t) - \Phi(x_i, t)] dt,$$

$q = (q_1, q_2, \dots, q_M)$, and $P_i, i = \overline{1, N}$ are the weights of measurements.

The dependence given by Eqs. (5) and (6) is the linear regression with respect to the vector θ . For the optimum planning of observations it is sufficient to use the methods proposed in Ref. 4.

Figure 1 shows optimum design for observations for the system of linear ground-based sources of pollution.⁵ The points of local maxima of variance of the near-ground concentration field are the points of the optimum disposition. As shown in Fig. 1 these are the points of intersection of linear sources.

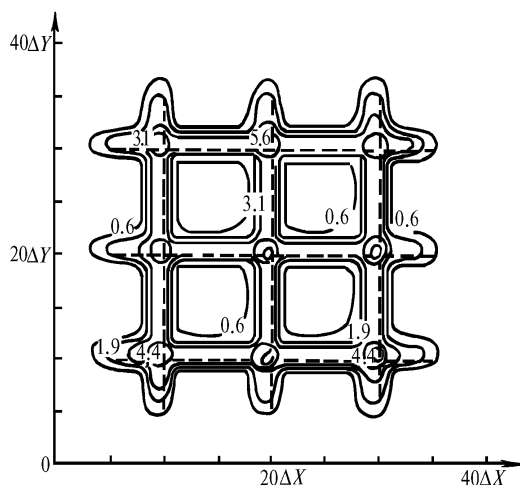


FIG. 1. Trace of variance matrix of near-ground concentration field (dashed lines correspond to source locations).

B. Determination of location and capacity of a source

Both the capacity of a source θ and its location X are the sought parameters. In this case the regression function is given implicitly, and a numerical solution of the problem (1)–(3) is required for its determination. The optimum design of observations depends nonlinearly on the parameters θ and X , and only its local representation is possible.

The search of optimum local design is realized by the following procedure of sequential designing⁶:

- 1) The search experiment is carried out using the plan $\varepsilon_N, \varepsilon_N$ is chosen from the condition of nondegeneration of the Fisher matrix.
- 2) Then estimations of $\hat{\theta}$ and X are calculated according to this plan by the least-square method.
- 3) The point

$$x_{N+1} = \text{Arg sup } d(x, \varepsilon_N, \hat{\theta}, \hat{X})$$

is then found, where $d(x, \varepsilon_N, \hat{\theta}, \hat{X})$ is the variance of the concentration field.

- 4) The additional observation is carried out at the point x_{N+1} . Then the operations from second to fourth are repeated.

The solution of the inverse problem on determining the source parameters θ and X is simplified when we use the property of dual representation of a linear functional depending on the concentration using direct and conjugate equations of pollutant transport.

Figure 2 presents an example of the solution of the inverse problem. Isolines of the goal function are shown in this figure. The source location coinciding with the minimum of the goal function is denoted by the asterisk, and the positions of observation points are marked with squares.

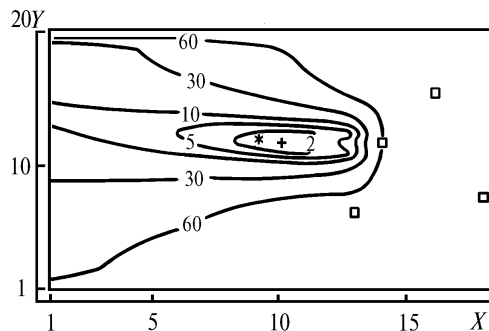


FIG. 2. Isolines of goal function: \blacksquare corresponds to location of observation points, * – to actual location of a point source, and + – to reconstructed location of a point source.

C. Reconstruction of the near-ground pollutant concentration

The inverse problem on reconstruction of aerosol pollutant concentration using the sparse observation network is considered for the sources located in the near-ground atmospheric layer. The solution of the problem (1)–(3) under the assumption of the power approximation of wind profiles and turbulent exchange coefficients is represented in the form of the nonlinear regression function of three parameters. Locally optimum observational plans for a light and heavy pollutants are constructed analytically and numerically using the above described procedure of sequential designing.^{9,10} Effective numerical algorithms for the determination of parameters of the regression function are developed.

Results of the reconstruction of density of aerosol sedimentation on vegetation using plans close to the optimum ones are presented in Fig. 3.

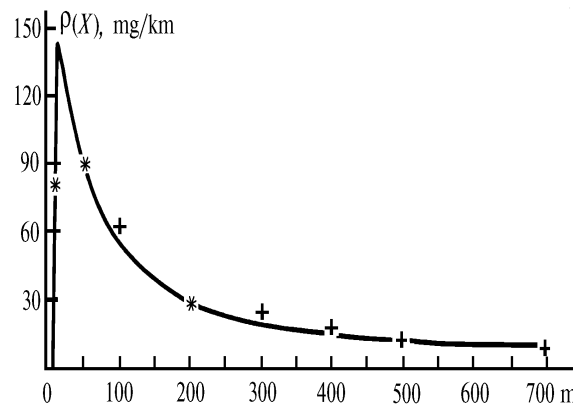


FIG. 3. Reconstructed sediment density of polydisperse aerosol on wheat: * and + correspond to data of density measurements and * – to measured density at points of sampling corresponding to the points of plan.

2. CONTROL OF AEROSOL SOURCES IN THE GROUND ATMOSPHERIC LAYER

Density of sedimentation, the amount of aerosol, summary function of potential losses and the cost for spraying, and so on can be used as criteria of effectiveness of aerosol spraying depending on the objectives pursued. In this case there appears a broad spectrum of the mathematical formulation of optimization problems.

A. The standard problem of aerosol technology

The usual aim of treatment of agricultural crops is the reduction of the aerosol amount per unit area. This is justified both by high cost of aerosols and requirements to the cleanness of the environment. However, the reduction of the amount of aerosol must not influence the effectiveness of its action. So, the optimization problem that arises can be formulated in the following way:

$$Q \rightarrow \min_d, \tag{8}$$

$$B(x, z, Q, d) \geq LD m, \quad x \in (0, l), \quad z \in (z_1, z_n), \tag{9}$$

$$q(l, z, Q, d) \leq q_{MPC},$$

where Q is the amount of aerosol used, B is the dose of aerosol taken by a pest during the treatment, LD is the lethal dose, m is the insect mass, l is the field depth, (z_1, z_n) is the vegetation layer, q is the concentration of aerosol, and q_{MPC} is the maximum permissible concentration.

Table I gives the numerical solution of the standard problem of aerosol technology.¹¹ This solution qualitatively agrees with knowledge of the behavior of the optimal parameters of the aerosol treatment.

TABLE I. Distribution of optimal amounts and diameters of aerosol particles for $R = 5$.

l , m	$Q_i/d_i, \text{ g/m}/\mu\text{m}, i = \overline{1, 5}$					Φ , g/m
	1	2	3	4	5	
500	23.6/20	5.3/21	5.9/22	5.7/24	5.7/30	46.3
1000	35.4/17	13.1/18	12.2/19	12.1/20	12.1/22	85.0
2000	60.1/16	32.7/16	30.4/16	28.3/17	28.2/18	179.8

B. The wave method

A possibility of additional reducing the amount of aerosol need for treating agricultural areas by using a more rational location scheme of aerosol sources. This is achieved by means of the optimum distributions of sources both with height and in the horizontal direction.

Table II gives the results of the use of the wave method when the aerosol generator moves across the wind direction. This method makes it possible to reduce additionally the amount of aerosol by more than half for some variants of spraying.¹²

TABLE II. Distribution of optimal amounts in treating by aerosol particles of equal diameter, $R = 5$.

l , m	α , μm	$Q_i, \text{ g/m}, i = \overline{1, 5}$					Φ , g/m
		1	2	3	4	5	
500	21	22.5	5.8	6.6	6.5	6.4	47.8
1000	18	33.3	14.0	13.5	13.0	12.8	86.6
2000	16	61.1	32.7	30.5	29.4	28.8	181.5

In solving the problem on the optimum source location with height, fitting the size of aerosol particles and the amount of aerosol at each level, it is possible to obtain the distribution of the sediment density that is close to the required one.¹³

C. Optimization of aerosol treatment in the presence of forest belt

Forest belt, forest parcels, and bushes are the most interesting objects in aerosol sprayings. The mathematical model suggested in Ref. 14 was used for the description of the interaction of air flow with these obstacles.

A standard problem of aerosol spraying taking into account the presence of forest belt is considered in Ref. 15. The solution of this problem is represented in Fig. 4. Analysis of results shows that the dose of aerosol changes sharply behind the forest belt.

In conclusion it should be noted that there is a definite similarity between the mathematical formulation of optimum control and inverse problems. However, there are the fundamental differences also. As a rule, uniqueness of the solution is necessary for inverse problems. The problems of optimum control require the complete description of conditions and restrictions in order to select the required solution from the set of permissible ones.

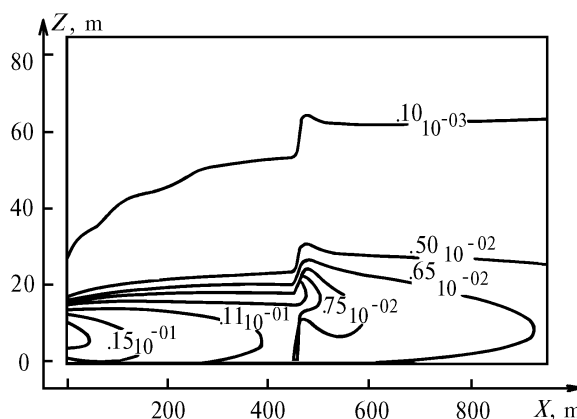


FIG. 4. Isolines of integral concentration of aerosol particles 2 μm in diameter in the presence of forest belt 10 m in height at $c_d s = 0.1 \text{ m}^{-1}$ (c_d is radiodynamic resistance coefficient, s is specific surface of vegetation elements).

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