Inverse problem of reconstruction of the density of aerosols precipitated on vegetation

T.V. Yaroslavtseva

Institute of Chemical Kinetics and Combustion,
Siberian Branch of the Russian Academy of Sciences, Novosibirsk

Received March 3, 1999

A number of models for estimating the density fields of precipitated aerosol preparations from measurements at a limited number of points is examined. The results of numerical experiments on reconstruction of the precipitated fields and aerosol parameters are presented for the models of light and mono- and polydisperse admixtures. The sensitivity of solutions of the inverse problems is investigated as a function of the arrangement of the measurement points.

Introduction

In the present paper, the problem of reconstructing the density of an aerosol preparation precipitated on vegetation is considered. The preparation was produced with an aerosol generator of regulated dispersity (GRD). For models of a light admixture and mono- and polydisperse aerosols three inverse problems are formulated on estimating the aerosol parameters and the density of the precipitated preparations from observations at different distances from the GRD emission axis. As the test function, we use the standard deviation of the measured and calculated precipitation densities. For light and polydisperse admixtures the measurable parameters are the effective source height and the interaction factor of the admixture with the vegetative cover. For monodisperse admixture the average sedimentation rate of the aerosol particles should also be determined.

To describe the spreading of an aerosol cloud, the semi-empirical equation of admixture transport for an instantaneous linear infinite source was used. The wind velocity and the vertical turbulent exchange coefficient are described by the Monin–Obukhov similarity theory. The basic input information in models for estimation of the density of precipitation are the distance of the sampling points from the source, the aerosol particle size spectrum, and the measured density of precipitation on the vegetation and soil. As additional information, the wind speed, the stability class of the atmospheric surface layer, etc. can be used.

Inverse problem formulation

The spreading of an aerosol admixture in the atmosphere from an instantaneous linear source located at the height H is described by the semi-empirical equation of turbulent diffusion[1]

$$u(z)\,\frac{\partial Q}{\partial x} - w\,\frac{\partial Q}{\partial z} = \frac{\partial}{\partial z}\,m(z)\,\frac{\partial Q}{\partial z} \qquad (1)$$

with boundary and initial conditions

$$m(z)\,\frac{\partial Q}{\partial z}\bigg|_{z=0,\,z=h} = 0,\quad u(z)\,Q\,\Big|_{x=0} = G\delta(z-H), \qquad (2)$$

where x and z are the horizontal and vertical coordinates, $Q(x, z)$ is the admixture concentration momentum, $u(z)$ is the wind speed (the x axis coincides with the wind direction), $m(z)$ is the vertical turbulent exchange coefficient, w is the rate of gravitational sedimentation of particles, h is the height of the atmospheric surface layer, δ is the delta-function, and G is the efficiency of the continuous linear source, in g/m.

To describe the meteorological parameters, the Monin–Obukhov similarity theory is used. Because the aerosol experiments were carried out for a stable surface atmospheric layer (at night time), in what follows we restrict ourselves to a mathematical description of just this case. The wind velocity profiles and the vertical turbulent exchange coefficient are given by

$$u(z) = \frac{u_*}{\chi}\left(\ln\frac{z}{z_0} + \beta\,\frac{z-z_0}{L}\right),\quad m(z) = \frac{u_*\,z}{1+\beta\,z/L}, \qquad (3)$$

where u_* is the dynamic velocity, z_0 is the roughness parameter, L is the Monin–Obukhov length, $\chi = 0.35$ is the von Karman constant, and $\beta = 4.7$.

For a stable atmospheric surface layer (night time), the empirical relation[2]

$$L = B\,u_*^2 \qquad (4)$$

is satisfied, where $B \approx 1100\ \mathrm{s^2/m}$.

The concentration momentum $Q(x, z)$ is related to the precipitation density by the expression

$$\psi(x, C, H, w) = C\,Q(x, z, H, w)\,\Big|_{z=h_0}, \qquad (5)$$

where C is the interaction factor of the admixture with the underlying surface, and h_0 is the height of the vegetation.

In problem (1)–(5) the unknown parameters are the velocity of gravitational settling of particles w, the source height H, and the factor C of interaction with the underlying surface. It is also required to establish the pattern of continuous spreading of the aerosol preparation with increasing distance from the source from the measurements of the precipitated aerosol density p_k, $k = 1, \ldots, N$ at the points x_k.

We introduce the following notation for the parameters to be evaluated:

$$S_1 = C, \quad S_2 = H, \quad S_3 = w, \quad \mathbf{S} = (S_1, S_2, S_3).$$

A solution to problem (1)–(5) is taken to mean an estimate of the vector **S** that minimizes the following quadratic functional:

$$J(\mathbf{S}) = \sum_{k=1}^{N} [\psi(x_k, \mathbf{S}) - p_k]^2 \to \min_{\mathbf{S} \in \Omega},$$

where

$$\Omega = \{C > 0;\ 0.5 < H \le 10\ \text{m};\ 0 \le w \le 0.1\ \text{m/s}\}. \qquad (6)$$

Methods of solution

A. Use of the conjugate equations of admixture transport

A solution of problem (1)–(6) of estimating the parameter vector **S** can be obtained by a method based on dual representation of the linear functionals of the concentration in terms of solutions of direct and conjugate problems of admixture transport.[3] The following chain of relations holds:

$$Q(x_k, S_2, S_3) = \int_0^h \int_0^X Q(x, z)\, \delta(z - z_k)\, \delta(x - x_k)\, \mathrm{d}x\mathrm{d}z =$$

$$= \int_0^h \int_0^X Q(x, z)\, L^* Q_k^*\, \mathrm{d}x\mathrm{d}z =$$

$$= \int_0^h \int_0^X Q_k^*(x, z, S_3)\, LQ(x, z)\mathrm{d}x\mathrm{d}z =$$

$$= \int_0^h \int_0^X Q_k^*(x, z, S_3)\, \delta(z - S_2)\, \delta(x)\, \mathrm{d}x\mathrm{d}z =$$

$$= Q_k^*(0, S_2, S_3), \quad k = 1, \ldots, N. \qquad (7)$$

Here, $x_k < X$, and Q_k^* is the solution of the following set of conjugate problems in the region $0 < z < h$, $x < X$:

$$L^* Q_k^* \equiv - u(z) \frac{\partial Q_k^*}{\partial x} + w \frac{\partial Q_k^*}{\partial z} -$$

$$- \frac{\partial}{\partial z} m(z) \frac{\partial Q_k^*}{\partial z} = \delta(x - x_k)\, \delta(z - z_k), \qquad (8)$$

$$\left(m(z) \frac{\partial Q_k^*}{\partial z} - w Q_k^* \right) \Bigg|_{z = 0,\, z = h} = 0, \quad Q_k^* \Big|_{x = X} = 0.$$

With Eq. (7) taken into account, functional (6) takes the form

$$J_N(\mathbf{S}) = \sum_{k=1}^{N} [\, S_1\, Q_k^*(x_k, z, S_2, S_3) \big|_{z = h_0} - p_k]^2. \qquad (9)$$

It should be noted that for light and polydisperse admixture the solution of the inverse problem is significantly simplified, because function (9) is specified in explicit form. For this purpose, it is sufficient to solve N conjugate problems (8).

B. Grid-point method

Because the accuracy of the observations used in the examined inverse problem is low (the errors in measuring the precipitation density may be as high as 10–15%), there is no need to solve them with very high accuracy. The low dimensionality of the posed problems and the uncertainty of the source function should also be taken into account. Hence it follows that it is expedient to apply the grid-point method, whose essence consists in calculating functional (6) or (9) on a discrete set $\Omega_1 \subset \Omega$ and searching for a minimum of the function $J(\mathbf{S})$ on this set.

In addition to simplicity of numerical realization of problem (1)–(6), another advantage of this approach is the possibility of finding of all local minima of functionals (6) and (9).

Numerical experiments

The precipitation density was measured at eight different distances x_i, $i = 1, \ldots, 8$ from the source, given in Table 1, for the following values of the parameters: the roughness parameter $z_0 = 0.05$ m, the source efficiency $G = 20$ g/m, and the wind velocity $u = 0.8$ m/s (at a height of 2 m). The dynamic velocity u^* was determined from the empirical dependence obtained for a stable atmospheric surface layer.

Approximation of a light admixture

We set the rate of gravitational sedimentation of the aerosol particles equal to zero. In this case, two unknown parameters must be determined, namely, the effective source height H and the interaction factor C with the vegetation.

To estimate these parameters, different pairs of reference observation points were selected from the above-indicated range of distances.

Results of reconstruction of the precipitation density from the densities at points x_1 and x_2 are presented in Fig. 1*a* and Table 1. An analysis of the results of numerical modeling reveals a systematic overestimation of the calculated dependence in comparison with the measured values of p_k at points x_3–x_8. This is explained by the fact that sedimentation effects were ignored in the model of admixture transport. The increase in the relative deviation of the calculated values from the observations with increase of the distance from the source emission axis should also be taken into account.

The calculated effective source height was 0.8 m and was much less than the actual value, which was 6–8 m (Ref. 4).

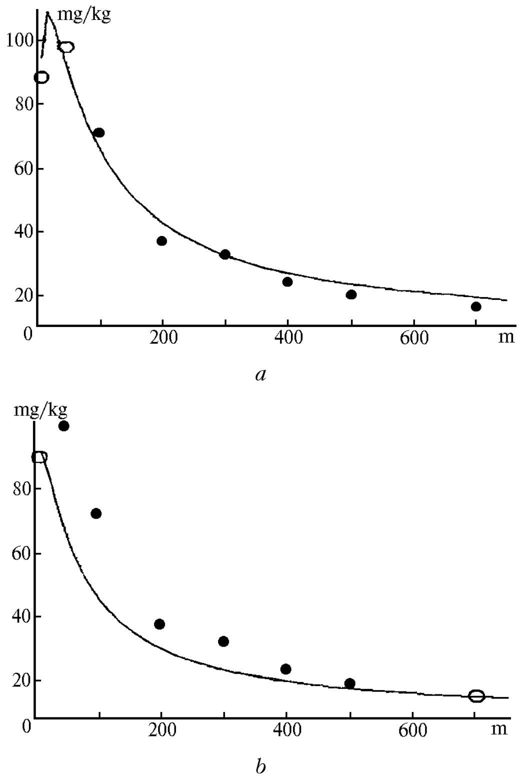

Fig 1. Reconstructed and measured densities of precipitated aerosols for a light admixture and observations at the points (x_1, x_2) (*a*) and (x_1, x_8) (*b*): calculated curve (solid line); measurements at the reference points (o); measurement test points (•).

On the whole, the result of reconstruction of the precipitation density may be considered satisfactory, and the given approximation can be used to estimate the upper limit of the sedimentation density.

To compare the accuracy of reconstruction, the results of a simulation of the precipitation density are shown based on the reference points x_1 and x_8. As our analysis demonstrates, this choice of the points is not entirely successful and demonstrates a higher sensitivity of the reconstruction to errors in the observations at these points.[5]

Monodisperse aerosol

For this variant of the model, it is necessary to specify, in addition to H and C, the average rate w of particle sedimentation from the aerosol cloud.

Estimation of the examined parameters requires the use of no less than three reference points (observation points). Our calculations were carried out for two sets of observation points: (x_1, x_2, x_4) and (x_6, x_7, x_8). Results of reconstruction of the unknown parameters and precipitation densities are presented in Table 1 and Figs. 2*a* and *b*.

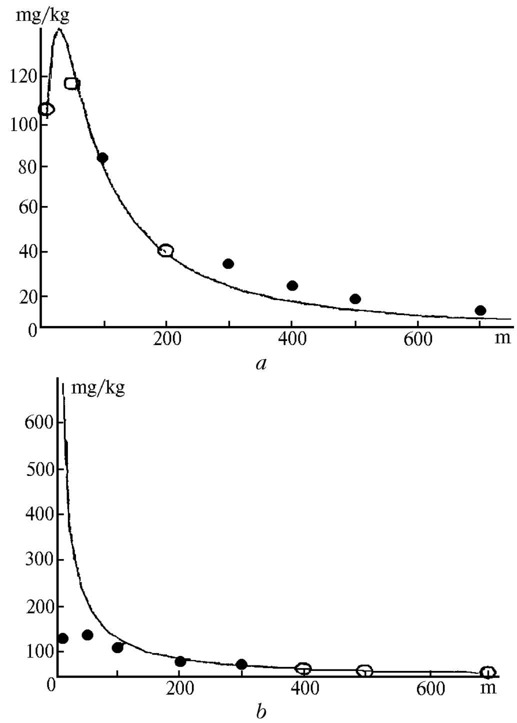

Fig. 2. Estimated precipitation density of the preparation for monodisperse aerosol observations at the points (x_1, x_2, x_4) (*a*) and (x_6, x_7, x_8) (*b*).

Our calculations demonstrate that gravitational sedimentation of aerosol particles leads to an increase in the effective source height to 2 m. On the other hand, taking the mechanism of admixture sedimentation into account leads to a more rapid decrease of the precipitation density in comparison with the experimental data. This circumstance allows us to use the model to obtain a lower estimate on possible sedimentations of the preparations.

Figure 2*b* shows an example of an unsuccessful choice of the reference points. The relative and absolute measurement errors at the sample points x_1–x_5 are very large, which is due to a suboptimal arrangement of the observation points.[4]

Table 1. Reconstructed and measured densities of precipitation on wheat, mg/kg.

Reconstruction model	Distance from the source, m							
	x_1 = 10	x_2 = 50	x_3 = 100	x_4 = 200	x_5 = 300	x_6 = 400	x_7 = 500	x_8 = 700
Light admixture	84.6*	82.1*	56.5	32.8	22.4	17.3	13.1	9.1
Monodisperse aerosol	76.4*	95.2*	58.3	26.1*	14.2	9.4	6.5	3.5
Polydisperse aerosol	81.3*	88.1*	59.4	33.2	22.0	16.1	12.0	8.4
Measurements	78.5	88	61	27	22.5	14.3	9.5	5.5

* For the measured precipitation density at the reference points.

Polydisperse aerosol

In the experiments we monitored the disperse composition of the aerosol particles, which is approximated with rather high accuracy by the lognormal distribution with the median-mass diameter $d_m = 12.7$ μm and geometrical standard deviation $\sigma_g = 2.6$.

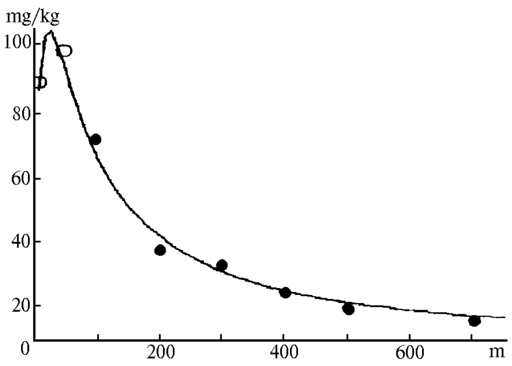

Fig. 3. Reconstructed densities of aerosols precipitated on vegetation in the polydisperse approximation.

Table 2. Estimated parameters of the inverse problems.

Reconstruction model	Source height, m	Sedimentation rates of aerosol fractions, cm/s	Interaction factor with the underlying surface, kg/m^2
Light admixture	0.8	0	134.6
Monodisperse aerosol	2	0.7	138.5
Polydisperse aerosol	3	0.01 0.06 0.13 0.23 0.37 0.6 1	37.4

Figure 3 and Tables 1 and 2 present the results of reconstruction of the precipitated aerosol density and the unknown parameters.

An analysis of the results shows that the effective source height increased to 3 m, which is explained by the presence of aerosol particles of heavy and light fractions in the aerosol particle size spectrum. As a consequence, the correspondence between the calculated and measured precipitation density of the preparation turned out to be fairly satisfactory at the sampling points x_3–x_8.

It should also be noted the relative error does not increase with distance from the source.

Conclusion

Based on the results of this study, we can conclude the following:

For light, mono-, and polydisperse admixtures the running parameters of the experiment have been estimated and the density of aerosols precipitated onto vegetation has been reconstructed from the data for a limited number of the observation points.

The set of reconstruction models used has allowed us to successively refine the aerosol source parameters and characteristics of the interaction of an aerosol admixture with vegetation, as well as estimate the maximum and minimum precipitation densities of the preparation.

The sensitivity of reconstruction of the precipitation density has been numerically investigated as a function of the arrangement of the reference points.

References

1. V.F. Dunskii, N.V. Nikitin, and M.S. Sokolov, *Pesticide Aerosols* (Nauka, Moscow, 1982), 287 pp.
2. F. Newstad and H. van Dop, eds., *Atmospheric Turbulence and Simulation of the Spreading of Admixtures* (Gidrometeoizdat, Leningrad, 1985), 351 pp.
3. G.I. Marchuk, *Mathematical Simulation as Applied to the Environmental Problem* (Nauka, Moscow, 1982), 320 pp.
4. V.V. Abramenko, A.E. Aloyan, A.N. Ankilov, et al., "*Numerical Modeling of the Spreading of Aerosols in the Atmospheric Boundary Layer above Vegetation,*" Preprint No. 584, Computing Center of the SB RAS, Novosibirsk (1985), 30 pp.
5. V.V. Fedorov, *Theory of an Optimal Experiment* (Nauka, Moscow, 1971), 312 pp.