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Assessment of fields of poly-disperse pollutants concentration in the vicinity of a distributed source*

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Abstract. The models of evaluating the mass and countable concentrations fields of aerosol pollutants in the vicinity of a distributed source were developed using a semi-empirical equation of turbulent diffusion in the surface atmospheric layer. With the models proposed, the fieldwork studies of the surface aerosol are numerically interpreted on lake Selitrennoe on the Altai territory, as an example.

1. Introduction

In conventional problems of transport and diffusion of aerosol pollutants in the atmosphere, the conditions for functioning of sources are assumed to be known. The situation is different in the case when the underlying surface is a pollutants source. Then the wind carrier of a pollutant and its subsequent transport will strongly depend on the state of this surface: humidity, grain-size analysis, sorption strength of a pollutant on the underlying surface, etc.). In its general statement, a solution to the wind migration problem presents a real challenge [1].

2. Fieldwork studies

As an object of analysis, lake Selitrennoe, located in the Western Altai, was selected. It represents an open reservoir of crystalline sodium sulfate of 6km area. Under certain meteorological conditions and technological processes, the discharge of a big part of sulfate particles of 0.05–10 µm into the atmosphere boundary layer is possible.

The location of the lake and a scheme of samples selection are shown in Figure 1. Aerosol samples were selected at 2 m height above the Earth's surface with the south-west wind. In 1997, the average wind speed in the samples selection was 6–8 m/s. According to the data gained in expeditions in 2004, the wind speed was somewhat lower, varying from 4 m/s up to 6 m/s. For defining the background, point 1 was located from the side of the lake exposed to the wind. As for observations at other points, they were made from the leeward side in the direction, coinciding with the wind.

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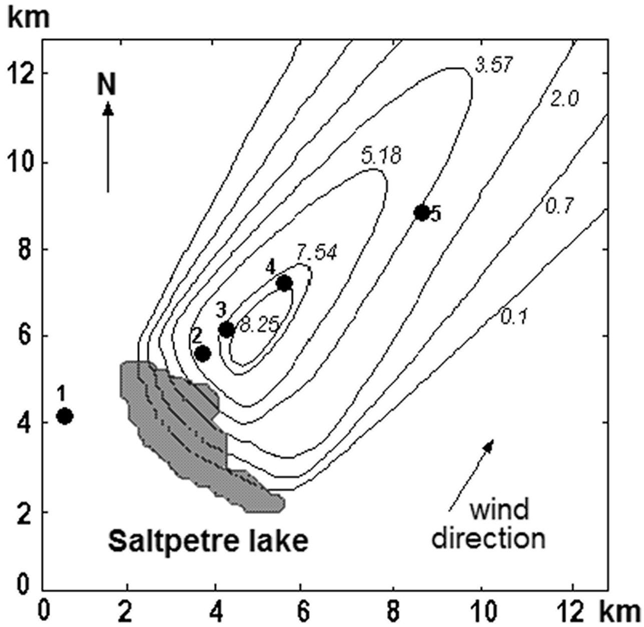

Figure 1. A scheme of the air samples selection. The restored field of the counting fraction concentration of 0.3–0.4 µm of sulfate aerosol in the vicinity of lake Selitrennoe. This field was formed with the south-west wind direction

Aerosol samples were selected at 2 m height over the Earth's surface with the south-west wind. In 1997, the average wind speed was 6–8 m/s. In the expeditions of 2004, the wind speed was somewhat lower and varied within 4–6 m/s. The fieldwork results have shown that sulfate aerosol from the surface of the lake in question is generated with the help of the two mechanisms: saltation and occurrence of spiral vortices. For defining the background, point 1 was located from the side of the lake exposed to the

Table 1. The measured values of the counting concentration (in thousands of particles/L)

Particles size, µm	Samples selection points / distance from the lake, km				
	1 / –	2 / 0.5	3 / 1.2	4 / 3	5 / 6
0.3–0.4	$\frac{1.16}{2.59}$	$\frac{5.25}{3.24}$	$\frac{7.89}{4.45}$	$\frac{8.25}{3.44}$	$\frac{3.88}{1.56}$
0.4–0.5	$\frac{1.16}{1.75}$	$\frac{6.32}{3.71}$	$\frac{6.3}{4.42}$	$\frac{7.05}{2.67}$	$\frac{4.29}{1.09}$
0.5–1.0	$\frac{0.74}{0.59}$	$\frac{3.35}{2.16}$	$\frac{2.47}{1.39}$	$\frac{1.19}{1.11}$	$\frac{1.59}{0.75}$
1–2	$\frac{0.04}{0.05}$	$\frac{0.67}{0.22}$	$\frac{0.37}{0.21}$	$\frac{0.06}{0.14}$	$\frac{0.02}{0.13}$
2–5	$\frac{0.02}{0.02}$	$\frac{0.21}{0.15}$	$\frac{0.14}{0.77}$	$\frac{0.02}{0.02}$	$\frac{0.01}{0.01}$

Remark. Measurements of 1997 in numerator via 2004 in denominator.

wind. Observations at other points were made from the leeward side of the lake in the direction, coinciding with the wind direction.

3. Statement of the inverse problems

Analysis of the available experimental data about aerosols concentration in the air, the observations system, the spatial-temporal structure of sources under study, the meteorological conditions show that the atmospheric pollution process should be preferably interpreted in terms of the statements of inverse problems of impurities transport. In this case, one should take account of availability of route observations, suitable surface orientation of dust sources as related to the prior directions of wind typical of the site under consideration.

The above-discussed information allows the use of superposition of concentration fields from a set of linear sources, which are located in the transverse to the wind direction, for the description of dust transport processes from a distributed source.

Approximation of a linear source. With the south-west wind, the concentration $q_\pi(r)$ at a distance r from a distributed source can be approximately calculated from the formula:

$$q_\pi(r) = \int_0^L q_l(r + L - \eta)\, d\eta, \tag{1}$$

where r is aligned with the direction of the wind, L is an effective width of a distributed source in the wind direction, $q_l(x)$ is the linear source concentration.

The impurities concentration in the air from a linear source is described with a semi-empiric equation of turbulent diffusion [2]

$$u(z)\frac{\partial q_l}{\partial x} - w\frac{\partial q_l}{\partial z} = \frac{\partial}{\partial z}m(z)\frac{\partial q_l}{\partial z}, \tag{2}$$

with the boundary and initial conditions

$$m(z)\frac{\partial q_l}{\partial z}\bigg|_{z=0,z=H} = 0, \quad u(z)q_l|_{x=x_1} = M\delta(z-H), \tag{3}$$

where z is a vertical coordinate, w is the deposition rate of aerosol particles, H is the effective height of the source, $u(z)$ is the wind speed, $m(z)$ is the vertical turbulent exchange factor, M is the power of the source.

When solving the inverse problems of aerosol propagation, the improvement can be gained by using analytical solutions to equation (2) for light and depositing impurities, i.e., approximating the functions $u(z)$ and $m(z)$ by power dependencies of the form [1, 2]:

$$u(z) = u_1\Big(\frac{z}{z_1}\Big)^n, \quad m(z) = \frac{k_1 z}{z_1}.$$

Here u_1 and k_1 are values of the wind speed and of the vertical turbulent exchange factor at a height of $z = z_1$.

In approximation of a sedimenting impurity, the analytical solution $q_l(x)$ has the following form [2]:

$$q_l(x) = \frac{M}{k_1(1+n)x^\omega}\exp\Big(-\frac{r_m}{x}\Big), \tag{4}$$

where

$$r_m = \frac{u_1 H^{1+n}}{(1+n)^2 k_1}, \quad \omega = 1 + \frac{w}{k_1(1+n)}.$$

Substituting formula (4) into (1) and using the theorem about the average from the integral computation, obtain

$$q_\pi(r) = \frac{ML\exp\Big(\frac{-r_m}{r+L-\lambda}\Big)}{k_1(1+n)(r+L-\lambda)^\omega}, \tag{5}$$

where $\lambda \in [0, L]$.

Carrying out in (5) the parameters aggregation procedure, we come to formula

$$q_\pi(r, \vec{\beta}) = \frac{\beta_1}{(r+\beta_2)^{\beta_2}}\exp\Big(\frac{-\beta_4}{r+\beta_2}\Big). \tag{6}$$

Here $\vec{\beta} = (\beta_1, \beta_2, \beta_3, \beta_4)$, $\beta_1 = \frac{ML}{k_1(1+n)}$, $\beta_2 = L - \lambda$, $\beta_3 = \omega$, $\beta_4 = r_m$.

In the general case, the vector of the parameters $\vec{\beta}$ can be estimated by the method of least squares employing the sequential analysis procedures and planning an experiment [9, 10]. Under certain assumptions, formula (6) can be reduced. In particular, for the light dust fractions at a low raising height and relatively large r and β_2, obtain

$$q_\pi(r, \beta_1, \beta_2) = \frac{\beta_1}{r+\beta_2}.$$

At large distances from a distributed source, the dependence on β_2 becomes weak. As a result we have

$$q_\pi(r, \beta_1) = \frac{\beta_1}{r}. \tag{7}$$

Approximation by point sources. Assume that the area of a source in question is approximated by the cover of N equal squares, corresponding to the action of a set of point sources of equal power. Let the axis x coincide with the wind direction, the axis y locating in the transverse direction. Then due to the superposition principle, the aerosol impurity concentration, formed by a distributed source, can be calculated from the formula [2]:

$$\Psi(x,y) = M \sum_{m=1}^{N} \frac{\exp\Bigl(\frac{-(y-y_i)^2}{2\phi^2(x-x_i)^2}\Bigr)}{\sqrt{2\pi}\phi(x-x_i)} q_i, \tag{8}$$

where $q_i = q(x-x_i)$ is the surface aerosol concentration, formed by a linear source that locates on the line $x = x_i$, M is the impurity emission per area unit, and ϕ is dispersion of the wind direction in a time of observations.

In the case of a weakly-sedimenting impurity ($\omega \approx 0$), the respective analytical solution to problem (2), (3) has the form

$$q(x-x_i,z)|_{z=0} = \frac{M\exp\Bigl(-\frac{u_1 H^{1+n}}{(1+n)^2 k_1(x-x_i)}\Bigr)}{(1+n)k_1(x-x_i)}. \tag{9}$$

Then with allowance for (8),(9) the surface concentration of a weakly-sedimenting impurity formed by a distributed source is described by

$$\Psi(x,y,\vec{\theta}) = \theta_1 \sum_{i=1}^{N} \frac{\exp\Bigl(-\frac{\theta_2}{x-x_i} - \frac{\theta_3(y-y_i)^2}{(x-x_i)^2}\Bigr)}{(x-x_i)^2} = \theta_1 Q(x,y,\theta_2,\theta_3), \tag{10}$$

where

$$\theta_1 = \frac{M}{(1+n)k_1\phi\sqrt{2\pi}}, \quad \theta_2 = \frac{u_1 H^{1+n}}{(1+n)^2 k_1}, \quad \theta_3 = \frac{1}{2\phi^2}. \tag{11}$$

Introducing of the vector of aggregated parameters $\vec{\theta} = (\theta_1, \theta_2, \theta_3)$ essentially decreases the number of unknown coefficients thus considerably reducing the problem of estimation. Estimations of the vector of the parameters $\vec{\theta}$ can be obtained with the method of least squares, using no less than three points of observations. In this case, the method of least squares is in finding the values of parameters that on a set of admissible values Ω provide with a minimum the functional

$$J(\vec{\theta}) = \sum_{k=1}^{K} \bigl[\Psi(x_k, y_k, \vec{\theta}) - r_k\bigr]^2 \to \min_{\vec{\theta}\in\Omega}. \tag{12}$$

Here r_k is a measured value of the impurity concentration at the kth point of observations.

With allowance made for the fact that θ_1 is linear in $J(\vec{\theta})$, functional (12) is written down as

$$J(\theta_1,\theta_2,\theta_3) = \sum_{k=1}^{K} [\theta_1 Q(x_k, y_k, \theta_2, \theta_3) - r_k]^2 \to \min_{\theta_1,\theta_2,\theta_3\in\Omega}. \tag{13}$$

The necessary condition of a minimum of functional (12) on the set Ω results in the relation

$$\frac{\partial J}{\partial \theta_1} = 2\sum_{k=1}^{K}[\theta_1 Q(x_k, y_k, \theta_2, \theta_3) - r_k]Q(x_k, y_k, \theta_2, \theta_3) = 0. \tag{14}$$

Then from equation (14), we obtain:

$$\theta_1 = \frac{\sum\limits_{k=1}^{K} r_k Q(x_k, y_k, \theta_2, \theta_3)}{\sum\limits_{k=1}^{K} Q^2(x_k, y_k, \theta_2, \theta_3)}. \tag{15}$$

Substituting (15) into data misfit functional (13), we arrive at an auxiliary problem of the search for a minimum of a function of the two variables θ_2 and θ_3, whose solution can be obtained using standard techniques of nonlinear programming such as the coordinate-wise descent method [11].

4. Numerical modeling

We analyze the observational data of mass concentration with the help of model (2). Figure 2 presents the results of restoration of the surface dust concentration in the direction of the sample selection route. Point 2 was taken as a reference point. A comparison between the calculations and observations at control points 3–5 reveals a sufficiently high level of agreement. An important indicator is a possibility of using dependence (2) to interpret the data of observations made both in 1997 and in 2004.

With the use of model (3), fields of calculated concentrations of different fractions of aerosol impurities were numerically restored with a limited number of observational points. For the given location of a system of sampling points, a characteristic value θ_3 was set for the daytime conditions [2].

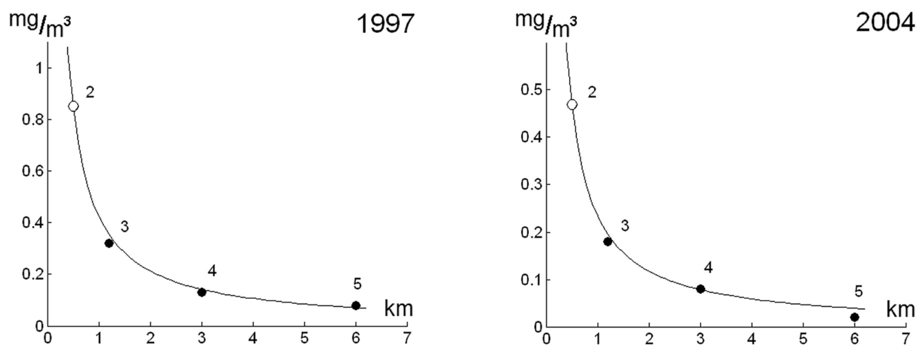

Figure 2. The measured and the calculated values of sulfate aerosol mass concentration. The horizontal axis indicates a distance from the lake along the route of observations. Solid line is a calculated curve; ○ and ● are measurements at a reference point and in control points, respectively

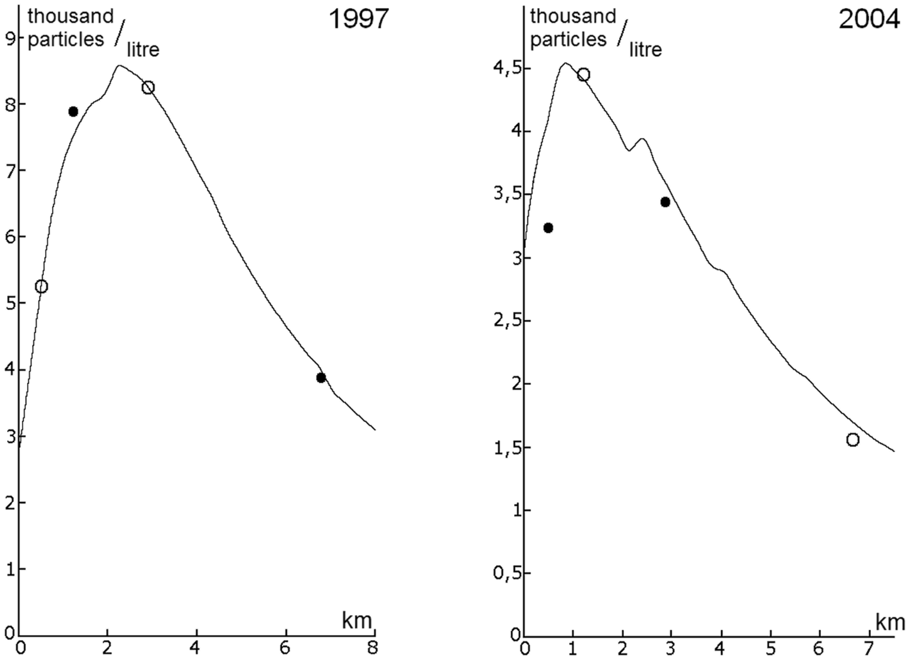

Figure 3. The measured and calculated concentrations for the fraction of 0.3–0.4 μm

The simulation results are shown in Figure 3. Estimations of parameters of model (10) are shown in Table 2.

The value of θ_2 distinctly varies with an increase of the particles sizes, which is directly associated with their effective ascent height above the lake surface. This circumstance indicates to the necessity of carrying out more thorough fieldwork studies dealing with distribution of the vertical concentration profiles for different sizes of particles and conditions of dusting the lake surface.

Table 2. Estimations of parameters of model (10) for observational data

Particles size, μm	1997		2004	
	θ_2, km	$\theta_1/10^6$	θ_2, km	$\theta_1/10^6$
0.3–0.4	2.5	4.24	1.4	1.01
0.4–0.5	2.3	3.51	1.0	0.81
0.5–1.0	1.2	0.91	0.8	0.25

5. Conclusion

The conducted theoretical analysis of the impurity propagation processes and the numerical investigation of data of fieldwork observations made possible to reveal the existence of sufficiently simple and stable regularities of aerosol contamination of the surface air layer from a distributed source. The quantitative models of restoring the fields of mass and calculated concentrations of sulfate aerosol appeared to be fairly adequate to observational data. The estimations presented show that effective ascent heights of particles of different fractions essentially depend both on their sizes and the wind speed. The obtained estimations of parameters make possible to numerically simulate the processes of sulfate aerosol propagation in the vicinity of the lake with an arbitrary wind direction for close states of dusting the lake surface and the turbulent exchange mode in the surface atmospheric layer.

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