DETERMINATION OF THE AEROSOL PARTICLE FLUX EMITTED FROM THE UNDERLYING SURFACE BY SOLVING INVERSE PROBLEM OF THEIR DISPERSAL IN THE ATMOSPHERE

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In this paper, the flux of aerosol particles from the underlying surface is estimated by solving the inverse problem of their dispersal in the atmosphere. The estimation method uses a conjugate equation of turbulent diffusion and the original model of aerosol dispersal in the boundary layer of the atmosphere. The results of the study of radionuclide lift by the wind in the Chernobyl accident zone and the measurement of the change of a weightless contaminants (methane) over a marsh are used as the initial data for practical examples. To reconstruct wind velocity profiles necessary for solving the turbulent diffusion equation, the data of standard meteorological observations were used.

The necessity of estimating the aerosol particle flux from the underlying surface arises when solving some practical problems, for instance, aerosol flux of sea salt or dust raised from the earth's surface. Usually, the emission of particles from the underlying surface is estimated by direct measurements, indirect methods, by data on a contaminant concentration over the underlying surface.[1] However, these approaches yield only local estimations in sufficient for obtaining integral emission parameters from large areas. Thus, the problem of estimation of the mean flux from large areas by values of contaminant concentration measured at some points over the underlying surface is important.

In this paper, we propose a method for estimation of a particle flux from the underlying surface by solving the inverse problem of particles' propagation in the boundary layer of the atmosphere. The method uses a conjugate equation of turbulent diffusion. The results of the study of wind rise of radionuclides in the zone of the Chernobyl accident[1] and the measurement of a weightless contaminant concentration (methane) evolved by a swampy underlying surface[2] were taken as the initial data.

Let the contaminant dispersal in the atmosphere be quasistationary and described by the semiempirical equation[3]

$$\bar{U}\frac{\partial\bar{C}}{\partial x}+\bar{V}\frac{\partial\bar{C}}{\partial y}+(\bar{W}-V_s)\frac{\partial\bar{C}}{\partial z}=\frac{\partial}{\partial x}(K_x+\nu)\frac{\partial\bar{C}}{\partial x}+$$

$$+\frac{\partial}{\partial y}(K_y+\nu)\frac{\partial\bar{C}}{\partial y}+\frac{\partial}{\partial z}(K_z+\nu)\frac{\partial\bar{C}}{\partial z}, \qquad (1)$$

where $\bar{C}$ is the mathematical expectation of the concentration; $\bar{U}$, $\bar{V}$, and $\bar{W}$ are the mean values of the wind velocity components $\bar{x}$, $\bar{y}$, and $\bar{z}$ respectively; V_s is the sedimentation rate of particles; k_x, k_y, and k_z are coefficients of turbulent diffusion; ν is the coefficient of molecular diffusion of particles. Let the x and y axes be in the horizontal plane, and the z axis be directed upwards. The assumption of quasistationarity of the diffusion process does not exclude the dependence of the coefficients in Eq. (1) on time.

Let us consider a spatial domain Ω including the underlying surface emitting aerosol particles and bounded by the planes $x = 0$, $x = X$, $y = 0$, $y = Y$, $z = H$, and the plane $z = 0$ corresponding to the underlying surface. Let S_0 be a part of the underlying surface emitting the particles. Let us also assume the following boundary conditions on Ω:

$$\bar{C}(0, y, z) = \bar{C}(X, y, z) = \bar{C}(x, 0, z) = \bar{C}(x, Y, z) =$$

$$= \bar{C}(x, y, H) = 0;$$

$$K_z\left.\frac{\partial\bar{C}}{\partial z}\right|_{z=0} = -\bar{q} \text{ on } S_0;\ K_z\left.\frac{\partial\bar{C}}{\partial z}\right|_{z=0} = 0 \text{ out of } S_0, \qquad (2)$$

where $\bar{q}(x, y)$ is the expectation of the contaminant flux.

According to Ref. 4, let us formulate the problem conjugate to Eqs. (1) and (2) in the form

$$-\bar{U}\frac{\partial C^*}{\partial z}-\bar{V}\frac{\partial C^*}{\partial y}-(\bar{W}-V_s)\frac{\partial C^*}{\partial z}=\frac{\partial}{\partial x}(K_x+\nu)\frac{\partial C^*}{\partial x}+$$

$$+\frac{\partial}{\partial y}(K_y+\nu)\frac{\partial C^*}{\partial y}+\frac{\partial}{\partial z}(K_z+\nu)\frac{\partial C^*}{\partial z}+R, \qquad (3)$$

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where $R(x, y, z)$ is some, not yet defined, function. Let us assume the following boundary conditions on Ω:

$$C^*(0, y, z) = C^*(X, y, z) = C^*(x, 0, z) =$$

$$= C^*(x, Y, z) = C^*(x, y, H) = 0;$$

$$K_z \left.\frac{\partial C^*}{\partial z}\right|_{z=0} = 0. \quad (4)$$

Let us multiply Eq. (1) by C^* and subtract Eq. (3) multiplied by $\bar{C}$, and integrate the obtained expression over the domain Ω. Taking into account Eqs. (2) and (4), we obtain

$$\int_{S_0} C^*(x, y, 0)\, \bar{q}(x, y)\, \partial x\, \partial y = \int_{\Omega} R\, \bar{q}\,(x, y, z)\, \partial x\, \partial y\, \partial z. \quad (5)$$

Let us assume that the surface emitting particles is homogeneous and q does not depend on x and y. Then, assuming R in the form

$$R(x, y, z) = Q\delta(x - x_0)\, \delta(y - y_0)\, \delta(z - z_0), \quad (6)$$

where Q is a constant, $\delta(\ldots)$ is the delta function, x_0, y_0, z_0 are the coordinates of the point in which the pollutant concentration is measured, we obtain

$$\bar{q} = Q\, \bar{q}\,(x_0, y_0, z_0) \left[\int_{S_0} C^*(x, y, 0)\, \partial x\, \partial y\right]^{-1}, \quad (7)$$

where $\bar{q}\,(x_0, y_0, z_0)$ is the measured value of concentration.

Thus, one can formulate the following algorithm of solving the inverse problem of determining the mean value of the pollutant flux. Assume that R has the form (6) at the point x_0, y_0, z_0, where the measured concentration is $\bar{q}\,(x_0, y_0, z_0)$. Without any loss of generality, suppose that $Q = 1$. Now, solving the conjugate problem (3) and (4), we obtain the Green's function C^* at all points of the domain Ω including the surface S_0. By Eq. (7), we obtain the unknown mean value $\bar{q}$ of the flux.

In Ref. 5, we justified the fact that the pollutant flux is proportional to the boundary value of the concentration expectation

$$\bar{q} = V\, \bar{q}\,(x, y, 0). \quad (8)$$

The factor V has the meaning of the characteristic linear rate of particle emission by the underlying surface and can be interesting when describing the emission process for concrete types of surfaces. The first results of estimation of the factor based on measurement data and calculations are presented in Ref. 5.

The direct and the inverse problem discussed above were solved numerically. For this purpose, a three-dimensional numerical model[6] describing the pollutant dispersal in a thermally stratified boundary layer of the atmosphere was used. The model is based on a linearized variant of a complete system of equations the boundary layer dynamics of the atmosphere and enables one to take into account nonstationarity of meteorological fields, and dynamical, thermal, and orographic inhomogeneities of the underlying surface.

The calculations by the model described above were performed using data from Ref. 1 in which the intensity of wind rise of a number of radionuclides from areas neighboring to the Chernobyl nuclear power plant was studied experimentally. We used the data obtained under horizontal homogeneity and averaged over three-day interval. On the average the thermal stratification of the atmosphere was neutral. So the obtained profiles of ^{144}Ce, ^{103}Ru, and ^{137}Cs concentration and wind velocity up to the height of 15 m were close to the logarithmic ones.[1]

In calculations, the profile of wind velocity and the coefficients of turbulent diffusion were reconstructed in correspondence with the average wind velocity at the height $z_0 = 2$ m by using numerical analytical models.[6] Then, the value $C(x_0, y_0, z_0)$, presented in Ref. 1 and normalized in the paper to $\bar{q}\,(z = 1$ m), was used for calculations of the flux by the algorithm discussed above.

Since in Ref. 1 the initial data were normalized by $\delta(z = 1$ m), the mean value of the flux was obtained normalized to the same value too. Below it is presented in conventional units. At the same time, this normalization, obviously, does not influence the rate of particle emission from the underlying surface.

Let us present the results which were calculated for $\bar{U}(z = 2$ m) = 3 m/s, neutral stratification, and $\bar{q}\,(z = 1$ m) = 1 conventional unit. The calculated values of the normalized radionuclide flux of the isotope ^{144}Ce and the characteristic rate of the particle emission by the underlying surface appeared to be equal to $1.6 \cdot 10^{-2}$ conventional units and $8.9 \cdot 10^{-3}$ m respectively.

The intensity of wind rise $\alpha = q/p$ and the empirical coefficient $\mu = \bar{q}\,(z = 1$ m)$/p$, where p is the density of aerosol sedimentation on the underlying surface, were also considered in Ref. 1. We calculated the ratio $\alpha/\mu = q/\bar{q}\,(z = 1$ m). According to Ref. 1, the value of α/μ averaged over five experiments equals $3.0 \cdot 10^{-2}$ m/s. According to our calculations, it is $2.5 \cdot 10^{-2}$ m/s. The coincidence is obviously satisfactory if one takes into account that the values of the parameters α and μ presented in Ref. 1, have a significant spread.

For making additional verification of the method, the calculations on estimation of a weightless contaminant flux (methane) were performed using experimental data obtained in the Bakchar rayon of Tomsk region at the Plotnikovo base of the Soil Science and Agricultural Chemistry Institute, Siberian Branch of the Russian Academy of Sciences. The Bakchar marshes were chosen as a subject of the study.[2] During the missions of 1994 and 1995, we performed hourly measurements of methane concentration, wind velocity, air temperature, and humidity over the marsh at the height $z = 2$ m from the underlying surface and at a distance of about 100 m from the border of the marsh. Meteorological measurements were performed using standard equipment.

The calculations were performed for the following values of the input parameters: $X = Y = 3000$ m, $H = 60$ m; the intervals of the difference grid were $\Delta x = \Delta y = 200$ m and $\Delta z = 2$ m. The marsh occupies about 6.6 km^2 of the area studied. Its border passes as a broken line from northnorthwest to southsoutheast. The chosen calculation grid at the side borders of which one should assign, according to Ref. 2, zero boundary conditions for $\overline{C}$ must yield errors in the concentration expectation because some of its boundary nodes are placed just over the marsh where the concentration does not equal zero. However, special calculations demonstrate that the border influence on $\overline{C}(x_0, y_0, z_0)$ is neglectable for the above-mentioned parameters of the model and the dimensions of the calculation domain.

Let us consider some results of the calculations. The calculated values of the methane flow on 26–27.07.94 and 17–18.08.95 are presented in the Fig. 1. The horizontal bars present the values of $\overline{q}$ measured by the chamber static method[2] (the length of a bar corresponds to the duration of the measurement process). One can see that the methane flux obtained experimentally changes smoothly, and the calculated values have a significant spread. It may be explained by the difference in time of air sampling (~1 min) and the averaging period in the measurement of the methane flux by the chamber-static method (~2 hours). The duration of meteorological observations was a few minutes.

In this situation, it is obvious that the temporal behavior of the methane flux measured by the chamber static method will be smoother as compared with the calculated values. However, the mean value $\overline{q}$ plus minus standard deviation obtained using chamber static method 17–18.08.95 was 300 ± 27 mgC/m^2·day, and the mean calculated value of the flux is 334 ± 150 mgC/m^2·day (the unit of the mass corresponds to the carbon mass contained in a methane molecule). According to the experimental data presented in Ref. 2, the flux value averaged over all the observations in 1992–1994 at the Bakchar marsh equals 221 ± 223 mgC/m^2·day, and the value calculated by the experiments on 26–27.07.94 is 154 ± 83 mgC/m^2·day. In general, taking into account the above remarks, the coincidence of the calculated and experimental values of the methane flux can be considered satisfactory.

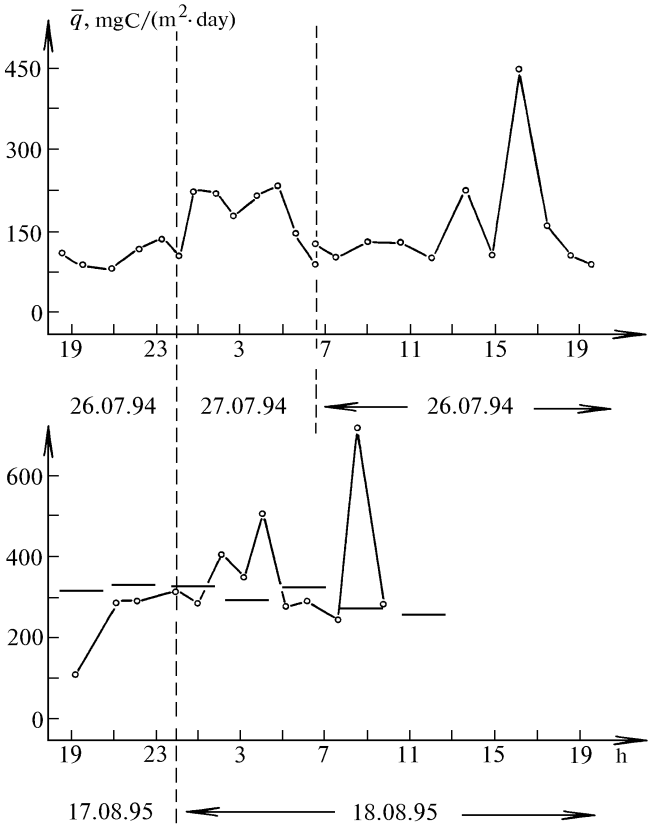

FIG. 1. The values of a weigthless contaminant flux (methane) obtained by the solution of the inverse problem.

When the methane flux was determined by the solution of the inverse problem (2) and (3), we used to solve the direct problem of the dispersal (1) and (2). The values of concentration $\overline{C}(x_0, y_0, z_0)$ obtained by calculation differ from the measured values no more than by 20%. Such a coincidence of the calculated and observed concentration values is rather satisfactory. This demonstrates the correctness of the proposed approach based on the solution of the inverse problem. In addition, this procedure demonstrates an acceptable accuracy of calculations reached in the application of numerical methods for the equations written above.

Let us consider the values of the characteristic linear rate of methane molecule emission by the underlying surface which were calculated by Eq. (8) in accordance of the data presented in the Figure. The mean value V for the experiment on 26–27.07.94 equals 5.5 ± 1.5 mm/s, and for 17–18.08.95 it is 4.9 ± 0.6 mm/s. We see that the mean value V

obtained approximately after a year at the same point of the marsh is in fact the same. Therefore, the relation (8) can be used for estimating the flux using the data on the nearground contaminant concentration.

Thus, the method for estimating the flow of the gas and aerosol contaminants from the underlying surface with the measured concentration values and the solution of the inverse problem can yield quite realistic values of a contaminant flux from the underlying surface.

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