

OPTICAL METHODS IN THE STUDY OF THE DYNAMICS OF THE ATMOSPHERIC BOUNDARY LAYER

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The fundamentals of the theory of optical monitoring of the surface boundary layer, performed for purposes of real-time remote sensing of the dynamical characteristics of the layer and subsequent solution of ecological problems of predicting pollutant transport, are presented. In particular, methods for solving the atmospheric-optical problem of constructing the field of the turbulent diffusion coefficients of aerosols from data obtained by laser sounding based on the scattering of light by the aerosol are discussed. The structure of the algorithm for determining the spatial-temporal variability of the aerosol microstructure field from optical measurements and for studying the physical processes involving aerosols under the conditions of a real atmosphere is given.

The spatial and temporal variability of the optical characteristics of aerosol in the atmosphere is determined by the diffusion transport of aerosol matter and transformation of the particle-size spectrum. Because of this situation remote sensing of aerosols based on the scattering of light can yield information about physical processes involving aerosols under conditions of the real atmosphere. This paper is devoted to the theory of such optical monitoring of the atmosphere performed for the purposes of studying the dynamics of the boundary layer. Knowing the dynamical parameters of the boundary layer it is possible to solve prediction problems associated with the emission of dispersed and gaseous pollutants into the atmosphere.

THE EQUATION OF ATMOSPHERIC DIFFUSION AND FORMULATION OF INVERSE PROBLEMS

The solution of the problem of predicting the transport of dispersed pollutants in the boundary layer usually involves the equation of atmospheric diffusion, which can be written in its general form as follows:

$$\frac{\partial Q}{\partial t} + \operatorname{div}(Q\vec{u}) = \operatorname{div}(\vec{D}\operatorname{grad})Q + \alpha Q, \quad (1)$$

where $Q(\vec{z}, t)$ is the concentration of transported pollutants (aerosols). Equation (1) contains, aside from the indicated function, the vector field of the wind velocity \vec{u} and the field of the turbulent diffusion coefficient \vec{D} .

The existing instrumentation for remote optical sounding of the atmosphere¹ as well as the computational methods for interpretation of the corresponding optical data^{2,3} permit determining the

concentration field of aerosol particles $Q(\vec{z}, t)$ and the vector field $\vec{u}(\vec{z}, t)$ with accuracy that is acceptable for many practical applications. This fact, naturally, leads us to formulation of a mathematical problem for Eq. (1) whose solution is the vector field of the diffusion coefficient $\vec{D}(\vec{z}, t)$. The practical significance of this is as follows. If the vector fields \vec{u} and \vec{D} are known at some moment in time, say, t' , within some local region of the boundary layer, then by solving the so-called direct problem for Eq. (1) for the scalar field $Q(\vec{z}, t)$, it is possible to predict the spreading of the pollutants at times $t > t'$. Prediction problems of this type constitute the principle content of what is customarily regarded as ecological monitoring of the environments.⁵ The investigation being conducted in this field are primarily oriented toward constructing some semiempirical a priori models for the vector fields \vec{u} and \vec{D} (Ref. 6).

The material in this article relies on the methods and instruments employed for optical monitoring and is based on the concept that reliable prediction of the ecological situation can be based solely on data from real-time remote sensing of the dynamical characteristics of the atmosphere. The basic theoretical aspects connected with the realization of this concept in the form of a computational theory of interpretation of empirical data are presented below.

In solving the diffusion equation (1) for the scalar field $Q(\vec{z}, t)$, the equation is usually reduced to a system of equations of the form

$$\frac{\partial Q}{\partial t} + \frac{\partial u_i Q}{\partial x_i} - \frac{\partial}{\partial x_i} D_i \frac{\partial Q}{\partial x_i} = c_i, \quad i = 1, 2, 3. \quad (2)$$

The choice of constants is usually conforms to the choice of scale factors, and without loss of generality they can be set equal to zero (see Ref. 7). The system (2) is constructed based on the so-called method of separation, applied in this case to Eq. (1).⁵ This method makes it much easier to solve the direct problem, i.e., the calculation of the field $Q(\bar{z}, t)$. In determining the field $\bar{D}(\bar{z}, t)$ the method is essentially equivalent to the separating Eq. (1) into partial equations for the unknown components $D_1 = D_x$, $D_2 = D_y$, and $D_3 = D_z$. Equations (2) are integrated in quadratures, and the computational aspects of this problem need not be discussed. The algorithmic apparatus that was developed for solving Eq. (1) for $Q(\bar{z}, t)$, can also be used to find the field $\bar{D}(\bar{z}, t)$. It is not difficult to show that the operator converting the set of initial data $\{Q, Q_t, \nabla Q\}$ into the vector \bar{D} is completely continuous and bounded (these questions are discussed in part in Ref. 8). Thus from the algorithmic viewpoint, the problem of determining the components of the field \bar{D} from Eq. (1) is virtually indistinguishable from the solution for the function $Q(\bar{z}, t)$. The separation into the direct and inverse problems here is more than symbolic, since these problems can be solved with the help of the same software, and, in particular, the software described in detail in Ref. 7.

It should be noted that to solve many practical ecological-monitoring problems it is sufficient to study simpler methods for determining the field of the turbulent diffusion coefficients. Thus in accordance with Ref. 6, instead of Eq. (1), a simplified version of this equation can be studied, namely,

$$u_x Q'_x - u_z Q'_z = \frac{\partial}{\partial z} D_z \frac{\partial Q}{\partial z} + \frac{\partial}{\partial y} D_y \frac{\partial Q}{\partial y} - \alpha Q. \quad (3)$$

Moreover it can be assumed that $D_x \approx D_y$ for altitudes of $z > h$, where h is the surface boundary layer. Then we can write Eq. (3) in the form

$$(a_1 D_x)' + (a_2 D_x)' = f, \quad (4)$$

where $a_1 = Q'_y$ and $a_2 = Q'_z$ and we denote by f the sum of remaining terms appearing in Eq. 3. Equation (4) can be further simplified by taking into account the fact that the z dependence of the function $D_x(x, y, z)$ can be approximated by a power-law function. A complete discussion of physically well-founded boundary conditions on the components of the field \bar{D} is given in Ref. 6. Mathematically it is much more difficult to solve the problem of determining the scalar field $Q(\bar{z}, t)$, its time derivative Q'_t , and the gradient ∇Q from data obtained by optical monitoring of the scattering component of the atmosphere. Methods for solving this problem are presented below.

THE THEORY OF OPTICAL MONITORING OF SPACE-TIME VARIABILITY OF THE MICROSTRUCTURE FIELD OF AEROSOL FORMATIONS IN THE ATMOSPHERE

It is convenient to start the analysis from an estimate of the field $Q(\bar{z}, t)$ from lidar data on aerosols in the boundary layer. The reason for starting the discussion with the method of laser sounding will be explained below, but for the time being we merely point out that $Q(z, t)$ is the concentration of particles whose sizes fall into the interval $[R_1, R_2]$. In the process of laser sounding the optical signal received from the atmosphere $P(\bar{z}, t, \lambda)$ is directly proportional to the backscattering coefficient $\beta_\pi(\bar{z}, t, \lambda)$. If the aerosols microstructure in a local volume is characterized by the distribution function of the particle volume over the particle size $v(r)$, then the backscattering coefficient can be written as follows:

$$\beta_\pi(\bar{z}, \lambda) = \int_{R_1(\bar{z})}^{R_2(\bar{z})} K_\pi[\bar{m}(\bar{z}), \lambda, r] \frac{3}{4r} v(r, \bar{z}) dr, \quad (5)$$

where K_π is a corresponding factor and m is the refractive index of the aerosol material.

In the problems of aerosol transport it is reasonable to assume $\bar{m}(\bar{z}) = \text{const}$, if, of course, over the period of optical monitoring there is not enough time for their chemical composition to change. Then the measured optical characteristic in the region sounded can be represented as a product $V(\bar{z}) \cdot \bar{K}_{\pi v}(\lambda)$, where $V(\bar{z})$ is the integral of the density $v(r, \bar{z})$ over the variable r within the indicated limits and $\bar{K}_{\pi v}(\lambda)$ is some average value of the factor in the integral (5). The assumption that the factor $\bar{K}_{\pi v}(\lambda)$ does not depend on the spatial coordinates makes it possible to regard it below as a constant whose value must be chosen a priori in an appropriate manner, after which the volume concentration field $V(\bar{z})$ is found from the lidar measurements of $\beta_\pi(\bar{z}, \lambda)$. Turning to Eqs. (2) it is not difficult to see that $Q(z)$ can be replaced not only by the volume concentration $V(\bar{z})$ but also directly by the field of the optical characteristic $\beta_\pi(\bar{z}, \lambda)$, since under the assumption adopted above $\beta_\pi(\bar{z}, t, \lambda) = V(\bar{z}, t) \bar{K}_{\pi v}(\lambda)$. How the not very trivial problem of determining $\beta'_{\pi t}$ and $\nabla \beta_\pi$ is to be solved will be described below. Thus we have shown that in the simplest interpretation the optical data from laser sounding of the aerosol component can be employed directly to invert the atmospheric diffusion equation in order to find the field $\bar{D}(\bar{z}, t)$.

There is nothing unexpected in this assertion, since the spatial-temporal variability of the concentration field of aerosol particles is directly manifested in the variations of the field of the aerosol optical characteristics. Of course, functionally, this relationship can be simple or more complicated. In this connection it should be noted that in the problem at hand the method of pulsed laser sounding has a significant advantage over other optical methods (geometric schemes). It lies in the fact that the lidar signal $P(\bar{z}, t, \lambda)$ received is essentially directly proportional to the characteristic $\beta_\pi(\bar{z}, t, \lambda)$ and in this sense the lidar method must be regarded as a direct method for determining $\beta_\pi(\bar{z}, t, \lambda)$.

In using different geometric schemes (path measurements of the spectral transmission, tangential sounding of the atmosphere from space, etc.) the determination of the optical characteristics of the atmosphere involves inversion of the integral radiation fluxes. For this reason the different optical methods of remote sounding must be regarded as indirect, if the problem is to determine the fields of the optical characteristics. This is what distinguishes the laser sounding method and makes it the single most important part of optical monitoring of the system "atmosphere-underlying surface", performed by the integrated optical instrumentation.⁹

A careful analysis of the approach presented above for studying the dynamics of the boundary layer from data obtained by optical monitoring shows that it is of an approximate (qualitative) character. It could possibly satisfy all the requirements associated with the solution of prediction problems in ecological monitoring of the dispersed pollutants; nonetheless it is possible to construct a more informative theory of optical investigations of the dynamics of the boundary layer, having in mind primarily, as done above, the determination of the vector field $\bar{D}(\bar{z}, t)$. Indeed any aerosol formation in the atmosphere consists of particles (fractions) of different sizes; this is characterized by the concept of aerosol "microstructure". In the above discussion it was connected with the distribution $v(r)$. In studying particle transport there is no harm in studying the transport of separate fractions, each of which contains particles with sizes r from the subintervals (r_l, r_{l+1}) ($l = 1, \dots, m$). We shall denote by $\Delta_l(V)$ the volume concentration of particles in the indicated fraction. It is obvious that if the density $v(r)$ is known, the following relation is satisfied:

$$\Delta_l(V) = v(r_{1+1}) - v(r_1), V(r) = \int_{R_1}^r v(r') dr',$$

$$l = 1, \dots, m \quad (6)$$

If data on $\{\Delta_l(V), (\Delta_l(V))'_t, \nabla(\Delta_l(V))\}$ were available to us, then we would be able to write an entire system

of equations of the type (2), each of which would describe the process of diffusion of the corresponding fraction. In order that this procedure for interpreting the microstructural data be of practical value strong physical foundations are required. One such foundation is that the turbulent diffusion coefficients of the particles depend strongly on the particle size. According to existing data,¹⁰ as the particle size r increases from 0.1 to 10 μm the coefficients D_l change by three orders of magnitude. For this reason, strictly speaking, we must consider the parametric field $\bar{D}(\bar{z}, t, r)$ in the starting equation (1). From the physical and mathematical viewpoints it is also important that the field \bar{u} is in no way connected with the parameter r and appears in Eq. (1) as an external factor. For this reason Eq. (1) can be regarded as a functional equation relating the partial distributions $\bar{D}(r|\bar{z}, t)$ and $v(r|\bar{z}, t)$. The interrelation of these two fields, on the basis of the approach studied here, forms the physical foundation for the study of the processes involving aerosol particle systems in the real atmosphere.

In order to have the required initial data for the inverse problem under study the volume of optical measurements must be increased. If we have in mind only the optical sounding (monitoring) instrumentation then it is reasonable to employ for these purposes multifrequency lidars first. When the measurement complex contains n working frequencies the lidar measurements give a collection of values of $\{\beta_\pi(\bar{z}, t, \lambda_i), i = 1, \dots, n\}$. When certain requirements, which will not be discussed here (see Refs. 2 and 3), are met this set of optical measurements can be converted into a set of microstructural data $\{\Delta_l(\bar{z}, t), l = 1, \dots, m\}$. However since the lidar measurements must be used to perform not only microstructural analysis of the aerosols but also to construct the gradients of the field of concentration of separate fractions we shall present the structure of the algorithm which transforms the collection of lidar data $\{P(\bar{z}, t, \lambda_i), i = 1, \dots, n\}$ in $\{\Delta_l(\bar{z}, t), (\Delta_l(\bar{z}, t))'_t, \nabla(\Delta_l(\bar{z}, t))\}$, where $l = 1, \dots, m$. We note that this algorithm can be used to solve not only the inverse problems of aerosol diffusion, but also the inverse problems of aerosol kinetics as a whole.⁸ Thus, in what follows we shall talk about the possibility of developing methods for studying physical processes in the atmosphere, relying on the availability of information obtainable in real-time by remote means. In order to employ this information, however, appropriate methods of interpretation are required.

To simplify the presentation we shall assume that the sounding is performed vertically and the determination of the gradient of the field $\Delta_l(\bar{z}, t)$ reduces to determining its derivative with respect to z . Assuming, as done previously, that the factors in Eq. (5) do not depend on the spatial coordinates, we shall write the expression

$$\frac{\partial \beta(z, \lambda)}{\partial z} = \int_{R_1(z)}^{R_2(z)} K(r, \lambda) \frac{\partial S(r, z)}{\partial z} dr, \tag{7}$$

or in operator form $\beta'_z = K S'_z$, where K is the integral operator corresponding to Eq. (7). We recall that $s(r) = \pi r^2 n(r)$, and we used the condition $s(r = R_1(z)) = s(r = R_2(z)) = 0$. As a result for any optical characteristic of the local volume, which depends on the spatial coordinate z and the time t , in the medium being sounded the following integral representation holds:

$$\beta = K_s, \quad \beta'_z = K S'_z, \quad \beta'_t = K S'_t \tag{8}$$

These integrals are inverted with the help of the same regularizing operator K_a^{-1} (Ref. 8). Since in the scattering atmosphere the formation of the lidar response is determined by two optical characteristics $\beta_\pi(z, t, \lambda)$ and $\beta_{ex}(z, t, \lambda)$, we shall require below the operator W which transforms the function $\beta_\pi(\lambda)$ into $\beta_{ex}(\lambda)$ for any optical sounding interval Λ . Formally this operator is defined as $K_{ex} K_\pi^{-1}$, where K_{ex} and K_π are integral operators with the kernels $K_{ex}(r, \lambda)$ and $K_\pi(r, \lambda)$, respectively.⁸ Under the same assumptions on which Eqs. (8) are based we can write

$$\beta_{ex} = W \beta_\pi, \quad \beta'_{ex,z} = W \beta'_{\pi z}, \quad \beta'_{ex,t} = W \beta'_{\pi t}. \tag{9}$$

In accordance with the theory of multifrequency sounding of the atmosphere based on the phenomenon of light scattering by aerosol^{2,3} the first operator in Eqs. (9), completing the determination of the equation describing the transfer of lidar signals in the spectral interval Λ , makes it fully determinate and uniquely solvable. But now we are faced with a complicated informational problem, since we are required to reconstruct from the lidar signal $P(z, t, \lambda)$ not only the field of the optical characteristics $\beta_{ex}(z, t, \lambda)$ and $\beta_\pi(z, t, \lambda)$, but also their derivatives. It is obvious that additional functional equations must be introduced in order to solve this problem uniquely. Before doing so, we recall that since the lidar measurements are performed only for a discrete set of wavelengths $\{\lambda_i, i = 1, \dots, n\}$ it is reasonable to put Eqs. (9) into a matrix form, i. e., to rewrite them from vectors, namely, $\beta_{ex} = \hat{W} \beta_\pi$ etc. The components of these vectors are the values $\beta(\lambda_i)$ ($i = 1, \dots, n$). When the lidar data are interpreted it is convenient to introduce the normalized function $S(z, t, \lambda) = P(z, t, \lambda) z^2 / B(\lambda) P_0(\lambda)$, where $B(\lambda)$ is an instrumental constant and $P_0(\lambda)$ is the power of the generated light pulse, instead of the lidar signal $P(z, t, \lambda)$.

Based on these remarks and starting from the lidar equation in single-scattering approximation we write the following relations:

$$\left. \begin{aligned} \beta_{\pi i} T_i &= S_i, \\ (\beta'_{\pi i z} - 2\beta_{\pi i} \beta_{1 \times, i}) T_i &= S'_{i z}, \\ (\beta'_{\pi i t} - 2\beta_{\pi i} \tau'_{i t}) T_i &= S'_{i t}, \quad i=1, \dots, n, \end{aligned} \right\} \tag{10}$$

where the following notation has been employed $\beta_{\pi i} = \beta_\pi(z, t, \lambda_i)$, $T_i = T(z, t, \lambda_i) = \exp\{-2\tau(z, t, \lambda_i)\}$,

$\tau(z, t, \lambda_i) = \int_{z_1}^z \beta_{ex}(z', t, \lambda_i) dz'$. Supplementing now the

system (10) with the matrix equations of the type (9), we obtain a fully determined system of functional equations for the functions $\beta_{\pi i}(z, t)$, $\beta'_{\pi i z}(z, t)$, and $\beta'_{\pi i t}(z, t)$. The functions found determine, through the system of operator equations (8), the field of the microstructure of the aerosol formation sounded and its space-time variability. The analytical constructions made above form the basis of the theory of optical monitoring of aerosol formations in the atmosphere, performed in order to monitor the space-time variability of the microstructure field. Analysis of the solvability of the equations falls outside the scope of this paper. We merely cite the work Ref. 2 where similar systems of nonlinear equations were studied in connection with the construction of a theory of multifrequency laser sounding of dispersed media. For practical applications the system of (9)–(10) must be put into a discrete form. To this end we shall make the system discrete in the variables z and t , by introducing the quantities $S_i^{(kv)} = S_i(z = z_k, t = t_v)$, $k, v = 1, \dots$, as well as the corresponding vectors $\vec{\beta}^{(kv)} = \{\beta_i^{(kv)} = \beta(z_k, t_v, \lambda_i)\}$, $i = 1, \dots, n$. Then the system of functional equations (10), solved beforehand for $\beta_\pi(z, t, \lambda)$ and its derivatives with the help of the relations (9), will assume the following discrete form:

$$\begin{aligned} \beta_{\pi i}^{(kv)} \cdot T_i^{(kv)} &= S_i^{(kv)}, \\ (\beta'_{\pi i z}^{(kv)} - 2\beta_{\pi i}^{(kv)} \cdot (\hat{W} \beta_\pi^{(kv)})_i) T_i^{(kv)} &= S'_{i z}^{(kv)}, \\ (\beta'_{\pi i t}^{(kv)} - 2\beta_{\pi i}^{(kv)} \cdot \tau'_{i t}^{(kv)}) T_i^{(kv)} &= S'_{i t}^{(kv)}, \\ \tau_i^{(kv)} &= \sum_{j=1}^k (\hat{W} \beta_\pi^{(jv)})_i \Delta_j(z), \\ \tau'_{i t}^{(kv)} &= \sum_{j=1}^k (\hat{W} \beta'_{\pi t}^{(jv)})_i \Delta_j(z), \end{aligned} \tag{11}$$

$i = 1, \dots, n, \quad k, v = 1, \dots,$

where $(\hat{W} \beta_\pi^{(kv)})_i$ denotes the quantity $\beta_{ex, i}^{(kv)}$, i.e., i -th component of the vector $\vec{\beta}_{ex}$, reconstructed from the vector $\vec{\beta}_\pi$ with the help of $n \times n$ matrix \hat{W} . In accordance with Eq. (8) the vector $\vec{\Delta}^{(kv)} = \{\Delta_i^{(kv)}, i = 1, \dots, m\}$, characterizing the microstructure field,

is determined with the help of the matrix operator \hat{K}_{α}^{-1} in the process of solving Eqs. (11). Such systems can be conveniently solved by iteration methods.² The matrix operator \hat{W} is calculated with the help of Mie's formulas. In order for the computational algorithm to be specified completely it remains to give a method for calculating the derivatives S'_z and S'_t from the empirical function $\tilde{S}(z, t, \lambda)$. Mathematically this problem has been studied well and, as is well known, it is an improperly posed problem. Since the function $\tilde{S}(z, t, \lambda)$ is in itself not differentiable, in the wider sense we are talking about how to construct for it a close analog that satisfies the required conditions that the analytic behavior be regular (differentiable). In application to the interpretation of lidar data the solution of this problem was presented previously in the monograph Ref. 3, so that we write out the final working formulas, making the system (11) complete in all respects.

As a simplification we introduce the notation $\varphi(z) = S_{lz}^{(v)}(z)$. It is obvious that

$$S_i^{(v)}(z) = S_i^{(v)}(z_1) + \int_{z_1}^z \varphi(z') dz'$$

The function $\varphi(z)$ is calculated in the following order:

$$\varphi_a(z) = \sum_{k=1}^q c_{ak} \chi(z, z_k), \quad (12)$$

where

$$\chi(z, z_k) = \begin{cases} 1 & \text{when } z \leq z_k, \\ 0 & \text{when } z > z_k. \end{cases}$$

The coefficients c_{ak} are found from the solution of the system

$$\sum_{j=1}^q a_{kj} c_j + \alpha c_k = \hat{f}_k, \quad k = 1, \dots, q, \quad (13)$$

in which

$$a_{kj} = \begin{cases} z_k - z_1 & \text{when } k \leq j, \\ z_j - z_1 & \text{when } k > j \end{cases}$$

and the right side $\hat{f}_k = \tilde{S}(z_k) - \tilde{S}(z_1)$. Once again α is the regularization parameter. It is clear that this sequence of calculations is based on an operator that transforms the empirical function $\tilde{S}(z)$ into its regular component $S_a(z)$, which has the required derivative with respect to z $S'_a(z)$. We recall that in the process of inverting the empirical data the regularizing algorithm simultaneously filters the noise (suppresses the irregular component of the empirical function). The algorithm constructed above solves the problem of writing the corresponding software for processing the data obtained by optical monitoring of the space-time variability of the aerosol microstructure fields, and combined with the equation of atmospheric diffusion (1) it gives a method for studying the dynamics of the surface boundary layer based on the scattering of light by the aerosol.

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