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Optical methods and algorithms for determination of fine aerosol parameters

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Abstract

An approach to diagnostics of aerosol media is suggested and relies on a developed hardware-software complex that combines two optical methods to measure disperse characteristics. This approach will make the measurements more informative (wider range of determinable sizes), which is of great practical importance for the environmental monitoring.

Keywords: Dispersiveness; spectral transparency method; small-angle method; Mie theory.

1. Introduction

Besides the urgent problems, mankind has now confronted the environmental challenge associated with natural and anthropogenic aerosol pollutions of community air. Aerosol is a hazardous contaminant to human health because particulates easily penetrate into the human organs while breathing. To monitor and develop effective techniques for sedimentation of the harmful aerosol, instruments are needed to identify particles in a wide size range.

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2. Optical methods for determination of aerosol dispersiveness

A great number of manufacturers from around the world offer their instruments for the diagnostics of fluxes, each of the instruments having its own drawbacks. These pertain to the particle size range, minimum and maximum concentration, cost, analysis time and so forth. Herein we suggest a mathematical and instrumental approach that would improve the performance of our measuring complex through the combination of devices and methods based on the devices. This promising approach on a basis of the developed hardware-software complex is of high practical significance for technology and industry and allows the combination of two optical methods for measurement of dispersed media' parameters (particle size and concentration distribution functions) in a wide size range (from 20 nm to 100 μm).

2.1 Small-angle method

Let us take a look at the existing measuring instrument that can determine parameters of aerosol media in the range of 1 to 100 μm (Fig. 1). This instrument relies on a modified method of small-angle scattering (Kudryashova et al., 2012) where the small-angle indicatrix of probe radiation scattering is recorded. The mathematical apparatus of the method consists in an assumption that the particle size and concentration distributions in an aerosol cloud are uniform.

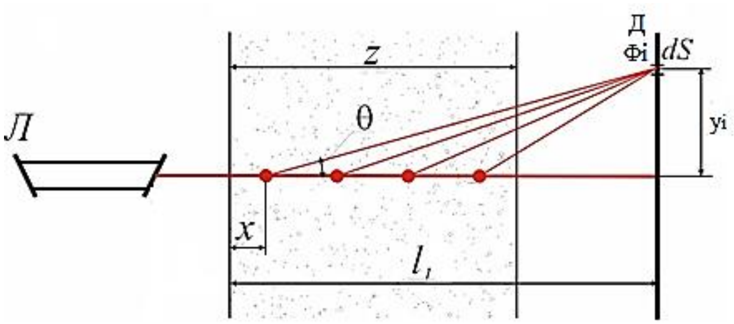

Fig. 1. The modified small-angle scattering method: Л – laser; x – step length; z – optical path length; Θ – scattering angle; l – distance from the border of the aerosol cloud to the photodetectors' plane; Д – photodetectors' plane; Φ_i – i-th photodetector; dS – photodetector area; y_i – distance from the optical axis to the photodetector.

The equation for the scattered radiation flux intensity (Shifrin, 1971) will take on the form:

$$I_{theor}(y_i) = \frac{\pi S C_n}{4} \int_0^z [I_0(x) B(x, y_i) F(x)] dx, \quad (1)$$

where S is the cross-section area of the probe beam; C_n is the calculated concentration; $I_0(x)$ is the radiation intensity at the distance x; $B(x, y_i)$ is the multiplier allowing for the scattered radiation attenuation;

$$F(x) = \int_0^\infty Q_s(D,\Theta)D^2 f(D)dD, \qquad (2)$$

where D is the particle diameter; Θ is the scattering angle; $f(D)$ is the particle size distribution function.

The intensity of the radiation incoming into the observation point:

$$I_0(x) = I_0 e^{-C_n \tau(x)}, \qquad (3)$$

where $\tau(x)$ is the optical depth depending on the optical path length.

The scattered radiation from a single particle for the small-angle region, when the particles are assumed to be spherical, is defined in the form of the analytic dependence:

$$Q_s\left(\frac{\pi D}{\lambda},\Theta\right) = \frac{\left(\frac{\pi D}{\lambda}\right)^2}{4\pi} \cdot \left[\frac{2J_1\left(\Theta\frac{\pi D}{\lambda}\right)}{\Theta\frac{\pi D}{\lambda}}\right]^2, \qquad (4)$$

where λ is the wavelength of the probe radiation; $J_1(\Theta\rho)$ is the first-order Bessel function of the first kind.

The multiplier allowing for the scattered radiation attenuation under the Buger's law is defined by the relation:

$$B(x,y_i) = e^{-C_n \tau \frac{z-x}{\cos\Theta(x,y_i)}}, \qquad (5)$$

where

$$\Theta(x,y_i) = arctg\left(\frac{y_i}{l_1 - x}\right). \qquad (6)$$

The gamma distribution was taken as the basic particle size distribution function:

$$f(D) = aD^\alpha e^{-bD}, \qquad (7)$$

where a is the normalizing factor; α, b are the distribution parameters.

The estimation of *f(D)* from the measured scattering indicatrix $I_{exp}(y_i)$ reduces to sweeping the parameters {α, b} of the distribution and to calculating the functional:

$$\Omega = \min_{\alpha,b}\left\{\sum_{i=1}^{n}\left|I_{exp}(y_i) - I_{theor}(y_i)\right|\right\}, \qquad (8)$$

where $I_{exp}(y_i)(i = 1,2,..,n)$ is the measured scattering indicatrix values for discrete positions on the plane; $I_{theor}(y_i)$ is the calculated indicatrix values.

2.2 High-selective turbidimetric method

We shall further consider the existing technique that enables characterization of aerosol media in the particle size range of 20 nm to 6 μm (Titov et al., 2012); its physical principle is based on the determinateness of the spectrum of the radiation passed through the medium under question in the wavelength range between 400 and 1100 nm, i.e., the disperse composition of the studied medium can be judged from the variation of the optical depth within the wavelength range measured.

In the high-selective turbidimetric technique, the particle size distribution function is estimated using the Fredholm equation of the first kind (van de Hulst, 1957):

$$I(\lambda) = I_0(\lambda) exp\left[-\frac{\pi C_n z}{4}\int_0^{\infty} Q\left(\frac{\pi D}{\lambda}, m(\lambda)\right) D^2 f(D) dD\right]; \quad (9)$$

where $I(\lambda)$ and $I_0(\lambda)$ are the intensities of the transmittied and incident lights passed through the aerosol medium at the wavelength λ at the moment of time t, respectively; $Q\left(\frac{\pi D}{\lambda}, m(\lambda)\right)$ is the attenuation efficiency factor; $m(\lambda)$ is the complex refrective index at the wavelength.

The particle size distribution function is then *a priori* introduced in the form of a generalized gamma distribution (7). The gamma distribution was chosen to describe the particle size distribution in view of its universality as applied to media with a single generation mechanism of the dispersed phase (van de Hulst, 1957); besides, this form of the particle size distribution is the most abundant in natural aerosols.

In solving the given problem, experimental information on the optical depth is exploited:

$$\tau_{\lambda} = ln\frac{I_0(\lambda)}{I(\lambda)}; \quad (10)$$

Afterwards, the relation of the optical depths at different wavelengths is to be found. The finding of the relation between the optical depths rather than their absolute values is done in order to enhance the estimation accuracy of the particle size distribution function by leaving out the multiplier $\frac{\pi C_n z}{4}$ before the integral sign in the formula (9) for the purpose of invoking less *a priori* information about the process under examination.

The relation between the optical depths for the corresponding wavelengths is further theoretically calculated for the specified particle size distribution function using precise formulae of the Mie theory.

The next step is to quantify the squared absolute deviation of the calculated value of the optical depth relations from the experimental. That form of the particle size distribution function is chosen which has the lowest deviation value.

3. Aspects of method combination

The combination of the two methods is feasible only when the specific features of each of these are taken into account. Each of the two has unique peculiarities which are due to physical and software implementation, measurement range, possibility to identify disperse characteristics with different optical wavelength, etc. The features of the high-selective turbidimetric (HST) and modified small-angle scattering methods (SAS) are given in Table 1. The final characteristics when combining the methods will be defined by the mutual intersection of their properties.

Table 1. Features of the optical measurement methods (HST and SAS).

HST	SAS
Particle size range 20 nm to 6 µm	Particle size range 1 to 100 µm
Measurement of aerosol parameters with optical depth up to 5	Measurement of aerosol parameters with optical depth up to 1.5
Measurement possible under background radiation	Measurements regardless of particle material
High optical path length, depending on particle concentration up to 2–5 m	Optical path length at most 1 m

In practice, when the methods are combined at the hardware level, the possibility of separately using each of the methods still remains, which provides flexibility upon determining the dispersiveness.

4. Hardware-software combination of the methods

At the mathematical level, we suggest an approach consisting in the replacement of the particle size distribution function (gamma distribution) by the vector (histogram). In doing so, we can obtain a histogram which will be able to describe experimental points more precisely (Fig. 2).

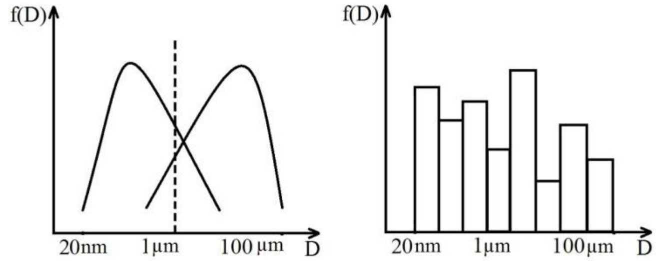

Fig. 2. Vector representation of the particle size distribution function.

The elaborated algorithms are currently based on solving a series of direct problems of aerosol optics. The theoretical and experimental processing of the methods requires considerable computational resources and is therefore practical only with the aid of a high-power computer. The theoretical implementation is embodied in the form of a software complex.

In summary, the suggested approach to diagnostics of aerosol media will help unite the two optical methods for dispersiveness measurement at the hardware-software level, significantly expanding the size range from 20 nm to 100 μm—which cannot be achieved with any existing instruments. In addition, the possibility to use each of the methods separately still remains.

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