EXPANSION OF THE SCATTERING PHASE MATRIX ELEMENTS OF THE ATMOSPHERIC HAZE OVER THE GENERALIZED SPHERICAL FUNCTIONS

A.B. Gavrilovich and V.I. Bychek

Physical Institute of the Academy of Sciences of Belarus, Minsk Received February 27, 1996

The expansion of the light scattering phase matrix elements over the generalized spherical functions is performed in order to determine the number of the expansion terms providing the representativity of calculational data in the problems on the transfer of polarized light. The expansion coefficients have been investigated assuming typical models of continental and urban aerosol. The model aerosol polydispersions involve, in certain proportions, such components as dust particles (insoluble in water), soluble particles, and soot particles. The data on the convergence of the diagonal and offdiagonal elements of the scattering phase matrices are presented.

INTRODUCTION

An enhanced interest has been shown in recent years in atmospheric observations using polarized light. This is connected with looking for new techniques for remote monitoring of the environment. Polarization effects, if used for atmospheric observations, provide much more information compared to simple scattering.¹ of development However, the corresponding polarization techniques is more difficult and requires a detailed study of the light scattering by methods of the transfer theory in a vector form. The vector transfer theory uses the expansion of the scattering phase matrix elements over the generalized spherical functions.^{2,3} It is difficult to take into account all the expansion terms, so one usually truncates the series to make engineering the calculations, restricting consideration to corresponding approximations. This paper deals with the expansion of the scattering phase matrix elements of atmospheric aerosol over the generalized spherical The number of terms to be taken into functions. account in order to provide the representativity of the data is assessed.

MICROSTRUCTURE AND OPTICAL PARAMETERS OF AEROSOL

The scattering phase matrix elements calculated by the Mie theory for various microstructure and optical constants of the aerosol make up the initial data set for the analysis. We use the models of the low atmospheric aerosols that are recommended by the Radiation Commission of International Association on Meteorology and Atmospheric Physics (IAMAP).⁴ Optical parameters of the aerosol substance are set, in the models considered, for the visible range. Each model includes the main aerosol components in certain proportions: D are water insoluble particles of soil origin (dust component); W are the soluble particles (ammonia, calcium sulfate, and organic compounds); and S are the carbon particles of anthropogenic origin. The aerosol components have their own refractive (n = 1.53(D); 1.53(W) and 1.75(S)) and absorption indices ($\varkappa \Box = \Box 8 \cdot 10^{-3}(D)$; $6 \cdot 10^{-3}(W)$, and $4.4 \cdot 10^{-1}(S)$) at the wavelength $\lambda = 0.55 \,\mu\text{m}$. Particle sizedistribution is approximated by a single mode lognormal distribution

$$f(r) = \frac{1}{\sqrt{2\pi\sigma r}} \exp\left[-\frac{\ln^2(r/r_0)}{2\sigma^2}\right],\tag{1}$$

where r_0 and σ are the parameters taking the values of 0.5 and 1.09527; 0.005 and 1.09527; 0.0118 and 0.69315 µm for the components D, W, and S, respectively. The modal radius $r_{\rm m}$ of the distribution is related to r_0 by the relationship $r_{\rm m} = r_0 \exp(-\sigma^2)$; mean radius is $\overline{r} = r_0 \exp(0.5\sigma^2)$.

Optical properties of a polydisperse ensemble of particles are mainly determined by the effective diffraction parameter $\rho_{32} = 2\pi r_{32} / \lambda$, where $r_{32} = r_0 \exp(2.5\sigma^2)$ is the effective radius equal to the ratio of the third and the second momenta of the particle size-distribution function. The value r_{32} of the dust particles (D) distribution is two orders of magnitude greater than that of the soluble particles (Wis equal to 10.033 and $0.1003 \,\mu\text{m}$, respectively). Carbon particles have the most narrow distribution and the smallest r_{32} value of 0.0392 μ m. The components D, W, and S presented in a certain proportion form the aerosol models analyzed in the paper. The proportion is 70% of D, 29% of W, and 1% of S by volume for the

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continental polydispersion and correspondingly 17%, 61%, and 22% for the urban aerosol polydispersion.

CALCULATION OF THE EXPANSION COEFFICIENTS OF THE SCATTERING PHASE MATRIX ELEMENTS OVER THE GENERALIZED SPHERICAL FUNCTIONS (GSF)

In the general case, to expand the scattering phase matrix elements $x_{ij}(\gamma)$ (γ is the scattering angle) over GSPs, it is necessary to replace the SP representation of the Stokes parameters with the CP-representation,⁵ in which the scattering phase matrix elements are expressed in terms of linear combinations of x_{ij} . In the case of spherical particles, $x_{11} = x_{22}$ and $x_{33} = x_{44}$. Therefore the analysis becomes simpler, and one can consider only two generalized spherical functions $P_{00}^{l}(\mu)$ and $P_{20}^{l}(\mu)$, where $\mu = \cos\gamma$. The functions $P_{00}^{l}(\mu)$ coincide with the Legendre polynomials, and $P_{20}^{l}(\mu)$ are expressed in terms of $P_{00}^{l}(\mu)$ (Ref. 6):

$$P_{20}^{l}(\mu) = -\frac{1}{\sqrt{(l-1)l(l+1)(l+2)}} (1-\mu^{2}) \frac{\mathrm{d}^{2} P_{00}^{l}(\mu)}{\mathrm{d} \mu^{2}}.$$
(2)

The coefficients of the scattering phase matrix elements expansion are calculated by the formulas

$$x_{l}^{11} = \frac{2l+1}{2} \int_{-1}^{1} x_{11}(\mu) P_{00}^{l}(\mu) d\mu,$$

$$x_{l}^{12} = \frac{2l+1}{2} \int_{-1}^{1} x_{12}(\mu) P_{20}^{l}(\mu) d\mu,$$

$$x_{l}^{34} = \frac{2l+1}{2} \int_{-1}^{1} x_{34}(\mu) P_{20}^{l}(\mu) d\mu,$$

$$x_{l}^{44} = \frac{2l+1}{2} \int_{-1}^{1} x_{44}(\mu) P_{00}^{l}(\mu) d\mu,$$
(3)

where the functions $P_{mn}^{l}(\mu)$ obey the condition

$$\int_{-1}^{1} |P_{mn}^{l}(\mu)|^{2} d\mu = \frac{2}{2l+1}.$$
 (4)

It is known that strongly oscillating behavior of the functions $P_{mn}^{l}(\mu)$ at large l causes unpredictable errors in calculations of the integrals (3). To resolve this problem, we have developed special procedure for calculating the integrals (3) for computations on an IBM PC/AT computer. Its idea is in linear interpolation applied to numerical integration of Eq. (3) at each part of the interval [-1, 1] for sufficiently smooth functions $x_{ij}(\mu)$, while the integrals of the strongly oscillating functions $P_{mn}^{l}(\mu)$ are calculated analytically with the use of recurrent formulas.

Integrating Eq. (3) by parts, the expressions for the expansion coefficients x_l^{11} and x_l^{44} are reduced to the form

$$x_{l}^{ii} = \frac{1}{2} x_{ii}(\mu) \left[P_{00}^{l+1}(\mu) - P_{00}^{l-1}(\mu) \right] \Big|_{-1}^{-1} - \frac{1}{2} \int_{-1}^{1} x_{ii}'(\mu) \left[P_{00}^{l+1}(\mu) - P_{00}^{l-1}(\mu) \right] d\mu.$$
(5)

Dividing the interval [-1, 1] into *N* small subintervals $\Delta \mu = \mu_{k+1} - \mu_k$ and using the linear interpolation of $x_{ii}(\gamma)$, the integral in the right-hand side of Eq. (5) is approximately replaced by a sum. Then we finally obtain for the diagonal elements:

$$x_{l}^{ii} = \frac{1}{2} \sum_{k=0}^{N-1} \frac{x_{ii}(\mu_{k+1}) - x_{ii}(\mu_{k})}{\mu_{k+1} - \mu_{k}} \times \left\{ \frac{1}{2l+3} \left[P_{00}^{l+2}(\mu_{k+1}) - P_{00}^{l+2}(\mu_{k}) \right] - \frac{4l+2}{(2l-1)(2l+3)} \left[P_{00}^{l}(\mu_{k+1}) - P_{00}^{l}(\mu_{k}) \right] + \frac{1}{2l-1} \left[P_{00}^{l-2}(\mu_{k+1}) - P_{00}^{l-2}(\mu_{k}) \right] \right\}, \quad i = -1, 4 \quad .$$
(6)

The expression for the offdiagonal elements $x_{12} = x_{21}$ and $x_{34} = -x_{43}$ can be obtained in a similar way, taking into account Eq. (2):

$$x_{l}^{ii} = \frac{2l+1}{2\sqrt{(l-1)l(l+1)(l+2)}} \sum_{k=0}^{N-1} \frac{x_{ij}(\mu_{k}) + x_{ij}(\mu_{k+1})}{2} \times \frac{l(l-1)}{l+1} \Big[\mu_{k+1} P_{00}^{l}(\mu_{k+1}) - \mu_{k} P_{00}^{l}(\mu_{k}) \Big] - \Big(l + \frac{2}{l+1}\Big) \times \Big[P_{00}^{l-1}(\mu_{k+1}) - P_{00}^{l-1}(\mu_{k}) \Big].$$
(7)

When deriving Eq. (7), we used the well known recurrent formulas 6 :

$$(1 - \mu^{2}) \frac{dP_{00}^{l}(\mu)}{d\mu} = -(l+1) \left[P_{00}^{l+1}(\mu) - P_{00}^{l-1}(\mu) \right],$$

$$P_{00}^{l}(\mu) = \frac{1}{2l+1} \left[\frac{d P_{00}^{l+1}(\mu)}{d\mu} - \frac{d P_{00}^{l-1}(\mu)}{d\mu} \right],$$

$$(8)$$

$$\mu P_{00}^{l}(\mu) = \frac{1}{2l+1} \left[(l+1)P_{00}^{l+1}(\mu) + l P_{00}^{l-1}(\mu) \right].$$

Linear interpolation gives a good approximation at a relatively low asymmetry of the scattering. The necessary accuracy is reached in the case of strongly elongated angular dependences by the Newton-Kotes method, by using the interpolating polynomials or the operation of the smooth additions to the functions $x_{ij}(\mu)$ in the range of small scattering angles.⁷ The estimate of the error in calculating the expansion coefficients obtained from the test calculations for the Heney-Greenstein scattering phase functions does not exceed 1% for l < 40 and reaches 10% for l > 140.

CALCULATIONAL RESULTS AND CONCLUSIONS

Angular behavior of the scattering phase matrix elements $x_{ij}(\mu)$ calculated by the Mie theory for a polydisperse system of spherical particles corresponding to the models of continental and urban aerosol are shown in Fig. 1. The comparison of solid and dashed curves shows that the dependences are qualitatively similar.

The differences are significant only in certain ranges of μ . The values x_{11} for continental aerosol in the range $\mu = 1$ (not shown in the figure) exceed the corresponding values for urban model by more than five orders of magnitude. The peculiarities in these aerosol models manifest themselves better in the representation by the terms of expansion, x_l^{ii} , over the generalized spherical functions. These differences are shown in Fig. 2*a* for $x_{11}(\mu)$ and $x_{44}(\mu)$. The solid and dashed curves correspond to the discrete spectra constructed for continental and urban aerosol, respectively, at integer *l*. The dependences for each aerosol model have two maxima (at l = 2 and $l \sim 140$); the ratio of maxima varies when passing from one model to another from the values essentially less than 1 to the values greater than unity. The calculations show (Fig. 2a) that the spectra x_l^{ij} for each separate component D, W and S are characterized by single mode distributions with the maxima at l = 1 (for the component S), 2(W) and 130-140(D). Obviously, the dual mode spectrum for the continental and urban aerosol models is explained by the decisive contributions from the components Wand S at small l values and from the component D at large ones.



FIG. 1. Scattering phase matrix elements for continental (solid curves) and urban (dashed curves) aerosol.

The most significant differences between aerosol models for the elements $x_{12}(\mu)$ (Fig. 2b) are observed at l values on the order of units, on the contrary, the differences for $x_{34}(\mu)$ are stronger in the range of large l values. That fact determines different convergence of

the corresponding series. The calculational results show that the observed oscillations of x_l^{12} and x_l^{34} gradually become weaker and then disappear as the refractive index *n* decreases and the absorption index \varkappa increases.



FIG. 2. Coefficients of expansion of the scattering phase matrix elements over the generalized spherical functions.

The quality of approximation of the scattering phase matrix elements $x_{ij}(\mu)$ by the truncated series was estimated according to two criteria. One is based on the closeness equation and by the rms deviation from the initial elements of the scattering phase matrix

$$x_{ij}(\mu) = \sum_{l = \sup(m,n)}^{L} x_l^{ij} P_{mn}^l(\mu)$$
(9)

at some L values. The first criterion uses Parceval-Steklov equality (closeness equation)

$$\sum_{l=\sup(m,n)}^{\infty} \frac{2}{2l+1} (x_l^{ij})^2 = \lim_{n \to \infty} x_{ij}(\mu) = \frac{2}{1-2}, \quad (10)$$

where $||x_{ij}(\mu)||$ is the norm of the scattering phase matrix element. The approximation quality is characterized by the value

$$\sum (L) = \frac{1}{\left\|x_{ij}(\mu)\right\|^2} \sum_{l=\sup(m,n)}^{L} \frac{2}{2l+1} \left(x_l^{ij}\right)^2.$$
(11)

It is obvious that $\Sigma(L = \infty) = 1$ in the case of the exact representation of $x_{ij}(\mu)$ by the series (9).

The rate of convergence of the series (9) for different elements of the scattering phase matrix is shown in Fig. 3. The deviation of $\Sigma(L)$ from unity of less than 1% is observed for continental aerosol at L > 200. The value L for urban aerosol is a little bit lower (about 160) but the rate of convergence is lower than that for continental aerosol model starting with $L \sim 5$.

The elements $x_{34}(\mu)$ have sufficiently good convergence even in the range *L* of 60, but the rate of

The results shown in Fig. 3 make it possible to obtain the number of expansion terms to be taken into account in the representation of the scattering phase matrix elements in the form of Eq. (9) for reaching certain preset deviation from the exact expansion. The value of deviation $1 - \Sigma(L)$ is usually determined by the requirements of the problem to be solved.



FIG. 3. Illustration of the convergence of series of expansion of different elements of the scattering phase matrix over generalized spherical functions.

The quality of approximation of the angular behavior of the elements of the scattering phase matrix $x_{ij}(\mu)$ by the truncated series (9) of the expansion over the generalized spherical functions is shown in Fig. 4. The data shown here are evidence of the fact that, taking, for example, 50 terms of the expansion over GSP, one can reach an acceptable accuracy of reconstruction of the angular behavior of the element $x_{44}(\mu)$ of the scattering phase matrix (Fig. 4*a*), while 10 terms are enough for correct representation of the behavior of $x_{12}(\mu)$ (Fig. 4*b*).

The data obtained in the paper and corresponding conclusions should be taken into account when solving the problems of optical radiation transfer in the atmosphere, considering polarization.



FIG. 4. Initial and reconstructed elements $x_{44}(\mu)$ and $x_{12}(\mu)$ of the scattering phase matrix for continental aerosol model.

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