PARAMETERIZATION OF THE AEROSOL SIZE-DISTRIBUTION FUNCTIONS FOR DIRECT AND INVERSE PROBLEMS OF ATMOSPHERIC REMOTE SENSING

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A technique for constructing the aerosol size spectrum correlation matrix based on the use of a number of analytic models of the stratospheric aerosol distribution is proposed. The feasibility of using such matrix eigenvectors as a model basis for the optical characteristics of a polydisperse aerosol is discussed, using the aerosol extinction coefficients as an example.

1. In order to solve the ill-posed inverse problems of atmospheric aerosol remote sensing, one has to state in some form the *a priori* information on the sought-after particle size spectrum, so that the retrieved function will be stable to random errors.

It is most natural to use statistical data for this purpose, since they reflect both the internal variability and the relation between the particle size intervals within the spectrum represented in the form of a correlation matrix of the particle size distribution function, the latter given as a histogram vs particle size. Using such a correlation matrix is also of interest in calculations of the reflected and scattered radiations, since this matrix makes it possible to estimate the variability of the natural aerosol extinction and scattering.[1] In the interpretation of lidar measurements the availability of the correlation matrix makes it possible to construct relations between the aerosol extinction and backscattering coefficients. The possibility of using the eigenvectors of the correlation matrix as a basis for approximating the aerosol size distribution functions should also be noted. Such an approach may serve as an engineering calculational technique for calculating the optical characteristics of polydisperse aerosols.

In this connection a heuristic approach is suggested below for constructing the correlation of the aerosol size distribution function based on certain analytic models of the stratospheric aerosol distribution.[5] Result illustrating the possibilities of its application to the solution of several of the above-mentioned problems are presented.

2. Let us consider a technique for constructing the model correlation matrix. We introduce the following abbreviated notation for the model distribution function borrowed from Ref. 5: $f_s(r,\ q_t\ ,\ p_k)$, where the indices have the following meaning: s prescribes the analytic form of the distribution function; r is the particle radius; q_t are the parameters estimated at some point; t is their number depending on s; p_k are the parameters prescribed base chosen measurement interval; k is the number of sub-intervals, into which the entire interval of variability for p_k is subdivided. The values of $f_s(r,\ q_t,\ p_k)$ employed in the computations are listed in Table I. It also lists the values of the parameter $\bar{X}$ which characterizes the ratio of the number of particles whose radius exceeds 0.15 μm to the number of those whose radius exceeds 0.25 μm ($N_{0.15}/N_{0.25}$) and σ is the standard deviation of this ratio, which is assumed to be a normally distributed random variable.

Computation of the distribution functions for all possible combinations of the above parameters makes it possible to form an *a-priori* model ensemble consisting, for example, of 900 model distributions, so that the ensemble average may then be obtained:

$$\bar{f}_i \equiv \bar{f}(r_i) = \frac{1}{L}\sum_{s=1}^{4}\sum_{t=1}^{T(s)}\sum_{k=1}^{100} f_s(r_i,\ q_t,\ p_k)w(s,\ t,\ k), \tag{1}$$

where $L = 900$, $T(s)$ is the number of parameters represented by their point estimates for the various distribution function (see Table I), and $w(s,\ t,\ k)$ is weighting factor. If $s = 4$ we treat q_t as a composite parameter (q_t', q_t'').

The i, j-th element of the correlation matrix of the particle size distribution function is computed from the thus constructed model ensemble as follows:

$$K_{ij} \equiv \bar{f}(r_i) = \frac{1}{L-1}\sum_{s=1}^{4}\sum_{t=1}^{T(s)}\sum_{k=1}^{100} w(s,\ t,\ k)\ \times$$
$$\times\ \left(f_s(r_i,\ q_t,\ p_k) - \bar{f}_i\right)\left(f_s(r_j,\ q_t,\ p_k) - \bar{f}_j\right), \tag{2}$$

where $w(s,\ t,\ k)$ is the weighting factor.

The values of $w(s,\ t,\ k)$ where determined assuming that for every s the maximum weight should be ascribed to those distribution realizations which are close to the respective averages given in Table I in their $N_{0.15}/N_{0.25}$ ratios. Taking into

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account the above assumption of a normal distribution for this ratio we may compute $w(s, t, k)$ from the following expression

$$w(s, t, k) = C \exp\left[-\frac{1}{2\sigma^2}\left(X_{s,t,k} - \overline{X}\right)^2\right], \qquad (3)$$

where C is a normalizing factor and $X_{s,t,k}$ is the computed value of the ratio $N_{0.15}/N_{0.25}$ for the respective realization of the size distribution function.

The proposed approach was applied to the spectral range from $\tau_1 = 0.01$ µm to $\tau_2 = 2$ µm, with the whole range uniformly divided into 30 sub-range over $\ln\tau$.

TABLE I. Model distribution functions $f_s(r, q_t, p_k)$ and parameters used to calculate the correlation matrix.

s	$f_s(r, q_t, p_k)$	Average values of the parameters q_t and p	Parameter p, range of variability
1. T=1	$\frac{A}{r\ln\sigma_g}\exp\left[-\frac{\ln^2(r/r_g)}{2\ln^2\sigma_g}\right]$	$p = r_g = 0.0725$ µm $q_1 = \sigma_g = 1.86$ $X = 4.9$, $\sigma = 3.7$	0.412–0.028 µm
2. T=0	$A\exp[-(r/r_0)]$	$p = r_0 = 0.075$ µm $\overline{X} = 3.8$, $\sigma = 2.6$	0.548–0.0361 µm
3. T=3	$A\exp\left[-\frac{\ln^2(r/r_m)}{2\ln^2\sigma_g}\right]$	$p = r_m = 0.035$ µm $q_1 = \sigma_g = 2.0$ $\overline{X} = 5.0$, $\sigma = 3.8$	0.263–0.011 µm
		$p = 0.1$ µm $q_2 = 1.8$ $\overline{X} = 2.7$, $\sigma = 1.5$	0.288–0.025 µm
		$p = 0.035$ µm $q_3 = 1.72$ $\overline{X} = 13$, $\sigma = 2$	0.296–0.035 µm
4. T=4	$Ar^{\alpha}\exp[-br^{\gamma}]$	$p = b = 20$ µm^{-1} $q_1' = \alpha = 2$ $q_1'' = \gamma = 1$ $\overline{X} = 3.4$, $\sigma = 2.2$	4.079–36.527 µm^{-1}
		$p = 18$ µm^{-1} $q_2' = 1$, $q_2'' = 1$ $\overline{X} = 4.1$, $\sigma = 2.6$	4.079–32.119 µm^{-1}
		$p = 8$ µm^{-1} $q_3' = 1$, $q_3'' = 1/2$ $\overline{X} = 3.2$, $\sigma = 2$	5.689–30.867 µm^{-1}
		$p = 16$ µm^{-1} $q_4' = 1$, $q_4'' = 1/2$ $\overline{X} = 3.2$, $\sigma = 2$	5.689–30.867 µm^{-1}

3. Let us now analyze the properties of the constructed model correlation matrix. Figure 1a gives, in relative units $\left(\sqrt{K_{11}}/\overline{f}_1\right)$, the diagonal of the matrix K, demonstrating the variability of the distribution function in the *a-priori* model ensemble for different particle size ranges. Note that such a variability attains its maximum at the boundaries of the considered range, reaching, in the same relative units, about 300% for $\tau \sim 2$ µm and about 150% for $\tau \sim 0.01$ µm. The values of the variability obtain for $r \sim 0.1$ µm (approximately 42%).

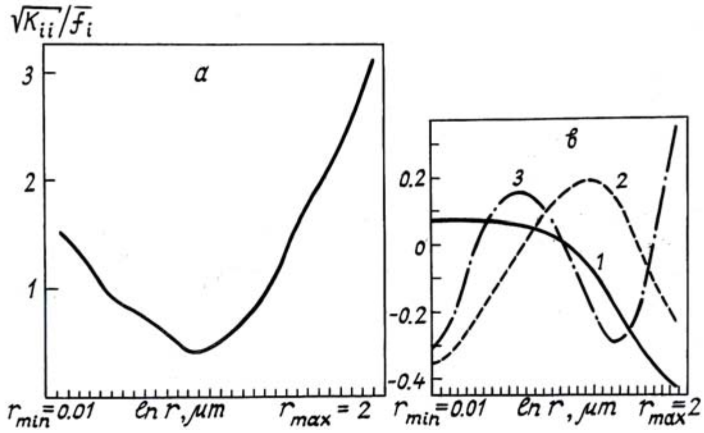

FIG. 1. The diagonal of the correlation matrix of the aerosol size distribution function (a) and the three first eigenvectors of the same correlation matrix (b).

TABLE II. Eigenvectors, eigenvalues, and the ensemble-average size distribution function

No.	1	2	3	4	5	6	7	8	$\bar{f}$
1	2	3	4	5	6	7	8	9	10
λ	42.7	10.9	4.93	2.21	0.753	0.234	8.62-2	2.45-2	
1	7.10-2	-0.354	-0.313	0.286	-0.231	-0.367	-0.341	0.244	3.61
2	7.13-2	-0.347	-0.282	0.216	-0.124	-0.116	-3.07-2	-7.87-2	4.03
3	7.12-2	-0.330	-0.236	0.129	-1.76-2	8.70-2	0.174	-0.223	4.51
4	7.06-2	-0.303	-0.176	3.30-2	7.80-2	0.219	0.256	-0.209	5.04
5	6.95-2	-0.269	-0.109	-6.24-2	0.153	0.273	0.226	-9.35-2	5.59
6	6.80-2	-0.231	-4.10-2	-0.146	0.199	0.255	0.124	4.66-2	6.10
7	6.60-2	-0.193	2.03-2	-0.209	0.212	0.184	-2.28-3	0.144	6.49
8	6.34-2	-0.154	7.13-2	-0.244	0.193	8.41-2	-0.108	0.162	6.67
9	6.02-2	-0.117	0.110	-0.250	0.146	-2.06-2	-0.162	9.45-2	6.59
10	5.61-2	-8.07-2	0.135	-0.227	7.65-2	-0.109	-0.151	-3.23-2	6.25
11	5.09-2	-4.42-2	0.147	-0.176	-6.07-3	-0.164	-7.79-2	-0.173	5.68
12	4.43-2	-7.51-3	0.146	-0.105	-8.86-2	-0.172	3.56-2	-0.276	4.98
13	3.63-2	2.91-2	0.133	-2.07-2	-0.156	-0.131	0.156	-0.297	4.22
14	2.66-2	6.45-2	0.109	6.47-2	-0.194	-4.62-2	0.243	-0.222	3.49
15	1.51-2	9.72-2	7.62-2	0.140	-0.191	6.26-2	0.265	-7.81-2	2.81
16	1.34-3	0.126	3.44-2	0.196	-0.145	0.168	0.209	7.70-2	2.20
17	-1.52-2	0.149	-1.50-2	0.226	-6.12-2	0.243	8.98-2	0.174	1.68
18	-3.52-2	0.167	-7.08-2	0.226	4.72-2	0.263	-5.68-2	0.164	1.24
19	-5.95-2	0.177	-0.131	0.196	0.160	0.215	-0.177	4.30-2	0.884
20	-8.84-2	0.178	-0.190	0.136	0.250	0.105	-0.216	-0.133	0.612
21	-0.122	0.169	-0.242	5.09-2	0.289	-3.85-2	-0.146	-0.263	0.412
22	-0.159	0.148	-0.276	-4.74-2	0.256	-0.166	1.20-2	-0.254	0.270
23	-0.198	0.116	-0.286	-0.142	0.151	-0.223	0.181	-8.98-2	0.173
24	-0.239	7.31-2	-0.266	-0.215	-4.39-3	-0.179	0.266	0.131	0.108
25	-0.279	2.25-2	-0.214	-0.248	-0.165	-4.56-2	0.205	0.254	6.49-2
26	-0.317	-3.35-2	-0.131	-0.228	-0.276	0.122	1.93-2	0.174	3.76-2
27	-0.352	-9.15-2	-2.22-2	-0.148	-0.288	0.239	-0.188	-6.62-2	2.09-2
28	-0.382	-0.148	0.104	-1.39-2	-0.170	0.224	-0.271	-0.273	1.11-2
29	-0.408	-0.200	0.236	0.158	6.68-2	4.24-2	-0.118	-0.208	5.61-3
30	-0.429	-0.246	0.362	0.340	0.373	-0.272	0.275	0.253	2.70-3

Note: $7.10^{-2} \to 7.10 \cdot 10^{-2}$.

Let us consider now the eigenvectors and eigenvalues of the constructed correlation matrix. The calculations demonstrate that such eigenvalues decrease quite rapidly: the sixth eigenvalue is two orders of magnitude less than the first one $\lambda_1 = 42.73$), and the eighth is another order of magnitude less. This result points to the possibility of employing a basis of the first six to eight eigenvectors to describe the complete *a-priori* model particle ensemble. Such a basis is referred to below as the "model" basis. Figure 1b gives the trends of the first three eigenvectors ($\lambda_1 = 42.73$, $\lambda_2 = 18.88$, $\lambda_3 = 4.93$) to illustrate the situation, and Table II lists the first eight eigenvectors and the corresponding eigenvalues, which reproduce the model correlation matrix with acceptable accuracy. The ensemble-average distribution function $\bar{f}(r_1)$ (1) is also shown.

The approximation capabilities of the constructed model basis were studied for both "adequate" distribution function (i.e., those entering the model ensemble) and inadequate ones.

As an example of an adequate distribution ($s = 3$ and 4, Table I), we considered the log-normal and gamma distributions, their parameter values corresponding to the "cleanest possible," "background," and "turbid" stratosphere. The "inadequate" functions were represented by bimodal log-normal distribution, with their second mode occupying different positions:

$$dN/d\ \ln r = \sum_{i=1}^{2} \frac{C_i}{\sqrt{2\pi}\,\sigma_g} \exp\left[-\frac{\ln^2(r/r_{m_i})}{2\sigma_g^2}\right]. \tag{4}$$

Such distribution function can be found in marine tropospheric aerosols.[3]

Figures 2a, b, c, d, e, and f plot the corresponding distribution functions and the results of their approximation in the model basis. These figures show that the constructed model basis approximates quite well both the adequate and the tested inadequate distribution. Larger approximation errors are found only in the tails of the single-mode distribution whose modal radii He at the boundaries of the intervals shown in Table I. It should be noted, however, that the values of the functions themselves in these tails are down by almost two orders magnitude in comparison with the maxima. Therefore this approximation errors should not be expected to play any significant role in the overall representation.

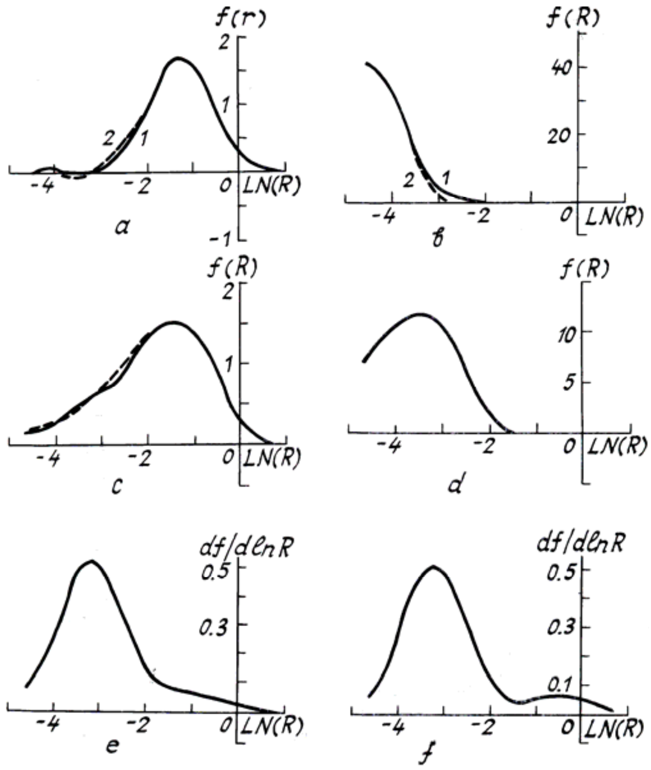

FIG. 2. Examples of approximations of various distribution functions in the model basis: the solid line is the "true" distribution; dashed line is the model approximation; a) s = 2 (see Table I), the parameters: $r_m = 0.263$ μm, $\sigma_g = 2$; *b)* $s = 2$, $r_m = 0.011$ μm, $\sigma_g = 2$; *c)* $s = 4$, $\alpha = 1$, $\gamma = 1$, $b = 4.079$; *d)* $s = 4$, $\alpha = 1$, $\gamma = 1$, $b = 32.119$; *e) bimodal distribution (see Eg. (4)) of* $\sigma_g = 2$, $C_1 = 0.9$, $C_2 = 0.1$, $r_{m_1} = 0.04$ μm, $r_{m_2} = 0.3$ μm; *f) bimodal distribution of* $\sigma_g = 2$, $C_1 = 0.9$, $C_2 = 0.1$, $r_{m_1} = 0.04$ μm, $r_{m_2} = 0.6$ μm.

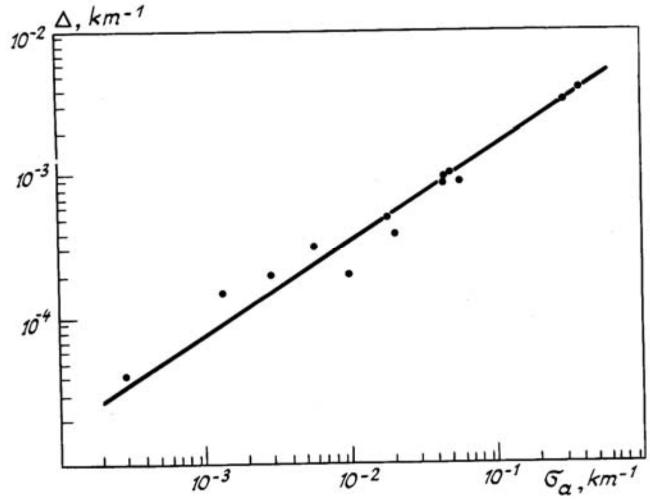

FIG. 3. Errors in the computed value of the extinction coefficient vs the coefficient itself.

4. Let us now assess the feasibility of using the constructed model basis to compute the optical characteristics of polydisperse aerosols, taking as our example their extinction coefficients. Taking into account the known relation (Ref. 2), we may use the following expression to compute such an aerosol extinction coefficient:

$$\alpha_{ex}(\lambda) = \sum_{i=0}^{8} b_i a_i(\lambda), \tag{5}$$

where b_1 are the expansion coefficients for the given function in the modal basis and $a_1(\lambda)$ is given by the expression

$$a_i(\lambda) = \int_{r_1}^{r_2} \pi r^2 Q_{ex}(r, m, \lambda) \bar{f}(r) \xi_i(r) dr,$$

$$i = 0, \ldots, 8,$$

where $Q_{ex}(r, m, \lambda)$ is the extinction efficiency factor for a particle of radius rand refractive index m at wavelength λ; $\xi_1(r)$ are the model basis functions: $b_0 = 1$, $\xi_0(r) = 1$.

Thus if we compute the coefficients $a_1(\lambda)$ for the given set of wavelengths λ, then obtaining the optical characteristics for a given refractive index does not require any additional Mie computations and is be reduced to computing the sum (5). Note that the described approach to computing the optical characteristics is close to the spectrozonal technique suggested in Ref. 4. However, in our case a more detailed representations of the distribution function is possible.

The accuracy of the approximation (5) in describing the extinction coefficients was tested for distribution function both adequate and inadequate to the model *a-priori* ensemble. The extinction coefficients were calculated at three wavelengths: $\lambda_1 = 0.3$, $\lambda_2 = 0.6$, 1.0 μm for the complex index of refraction $m = 1.44–0.01$.

Figure 3 shows the absolute calculational errors for the extinction coefficient $\Delta = \alpha^t_{ex} - \alpha_{ex}$, where α^t_{ex} is the extinction coefficient obtained by direct integration of the given distribution function, and α_{ex} is that same coefficient obtained using formula (5). The absolute errors Δ are presented versus α_{ex}, for a particle number density of 100 cm^{-3}.

We see that $\Delta(\alpha_{ex})$ illustrates the effect that the approximation errors in the particle size distribution function have upon the computed extinction coefficient. They are plotted vs the distribution modal radius. For bimodal distributions, this is essentially the dependence on the relative position of the two modes. Analyzing the data shown in Fig. 3 we see that the dependence of Δ on α_{ex} is close to linear, within the chosen interval of variability of α_{ex}, so that for the maximum values of $\alpha_{ex} \sim 0.4$ km^{-1} it does not exceed roughly 0.004 km^{-1}.

In conclusion we summarize the principal results of the described study.

1. A model correlation matrix has been constructed for the aerosol size distribution functions.

2. The approximational capabilities of the model basis, constructed for the first eight eigenvectors of this matrix, have been estimated. It has been shown that it approximates quite well both the functions adequate to the initial ensemble, and certain inadequate distributions.

3. The model basis has been shown to be usable for comparing aerosol extinction coefficients. The maximum computational errors do not exceed 0.004 km^{-1} for the considered distribution functions at a particle number density of 100 cm^{-3}.

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