

MODELS OF SIZE SPECTRUM OF TROPOSPHERIC AEROSOL

H. Tammet

Tartu State University, Ulikooli 18, Tartu, 202400, USSR

ABSTRACT

Quality criteria of a model distribution are considered. Information losses due to the nonorthogonality of spectrum-parameters transformation are discussed. Models are compared with a view to approximation accuracy and losses of information. Smerkalov's average tropospheric aerosol spectrum and 271 observed spectra have been used for test. Highest accuracy and lowest losses of information were yielded by the distribution $n_1(r) = a/((r/r_x)^k + (r_x/r)^l)$ having power asymptotes on both, the left and the right, sides.

QUALITY CRITERIA OF THE MODELS

Model distribution or model spectrum is a tool in the preparation of empirical data for making physical conclusions. It is a mathematical expression containing free parameters which enable us to fit the model to concrete data. In making physical conclusions information given through parameter values and estimates of measurement errors is used. The quality of the model depends on the losses in the transformation of initial empirical information into immediately manageable representation. There are three basic causes of such losses:

- 1) approximation errors due to inadequacy of the model,
- 2) uselessness of the information given through the coefficients of correlation between measurement errors of different parameters,
- 3) uselessness of the information given through parameters without actual interpretation.

The information losses due to the second cause deserve special attention.

A model spectrum can be described by a function $f(r, \vec{p})$, where r is the radius of the particle and $\vec{p} = (p_1, p_2, \dots, p_v)$ the vector of parameters. The quality of a nonlinear model depends on the set of spectra to be approximated. Let us consider the neighbourhood of a spectrum $\vec{n}^0 = f(\vec{r}, \vec{p}^0)$ given through the model with a certain vector of parameters \vec{p}^0 and a given vector of radii $\vec{r} = (r_1, r_2, \dots)$. If the empirical spectrum \vec{n} on the same set of radii is not far from \vec{n}^0 , then the respec-

tive values of parameters will be estimated with the linear algorithm of least squares

$$C = (B^T D^{-1} B)^{-1}, \quad \vec{p} = \vec{p}^0 + C B^T D^{-1} (\vec{n} - \vec{n}^0), \quad (1)$$

where D is the covariance matrix of the measurement errors of the spectrum \vec{n} and B is the Jacobi matrix with the elements $B_{ji} = \partial f(r_j, \vec{p}) / \partial p_i$ in the point \vec{p}^0 . C is the covariance matrix of the estimation of \vec{p} . The volume V_1 of the scattering ellipsoid of the parameter values describes the empirical information. This volume is proportional to $\sqrt{\det C}$. In physical analysis of observations each parameter gets its own individual meaning and will be considered separately. In this case we utilize the information described by the volume V_2 of an ellipsoid constructed on orthogonal axes having lengths proportional to the standard deviations of parameters $\sqrt{C_{jj}}$. The quantity of lost information is

$$\Delta I = \log(V_2/V_1) = \frac{1}{2} \left(\sum_j \log C_{jj} - \log \det C \right). \quad (2)$$

This is equivalent to the loss which we would have, if we multiplied all measurement errors by the factor

$$K = \left(\prod_j C_{jj} / \det C \right)^{1/2v}. \quad (3)$$

We call K the coefficient of error amplification due to the nonorthogonality of model.

THE CONSIDERED MODELS

The spectrum is described by the function $n_1(r) = dN/d \ln r = r dN/dr$, where N is the numerical concentration of particles with radii less than r. The models will be denoted by labels.

MG : $n_1(r) = ar^a \exp(-br^b)$ - a modified gamma-distribution.

S1A : $n_1(r) = ar^{-k} \exp(-br^{-s})$ - the "mirror" modification of MG.

MG and S1A as variants of one unitary model have been considered in [1]. A thorough analysis of S1A is given in [2].

S1B : $n_1(r) = a_1 (\hat{r}_1/r)^k \exp(\frac{k}{s}(1-(\hat{r}_1/r)^s))$ - a modification of S1A,

$\hat{r}_1 = (bs/k)^{1/s}$, $a_1 = ar_1^{-k} \exp(-k/s)$.

S2 : $n_1(r) = ar^{-k} \exp(-b/r-cr)$ - proposed in [3].

SME : $n_1(r) = a (\exp(-k(|r-\hat{r}_1|/r)^v)) / (\hat{r}_1^v + |r-\hat{r}_1|^v)$ - proposed in [4]. The spectrum described in this model

$$n_1(r) = a \cdot \exp(-0.42|1-0.03/(r:\mu m)|^{0.47}) / (0.000416 + |r:\mu m - 0.03|^3) \quad (4)$$

is close to the spectrum of tropospheric aerosols averaged from the data

given by various authors.

KLO : $n_1(r) = a / ((r/r_x)^k + (r_x/r)^l)$ - see the Figure.

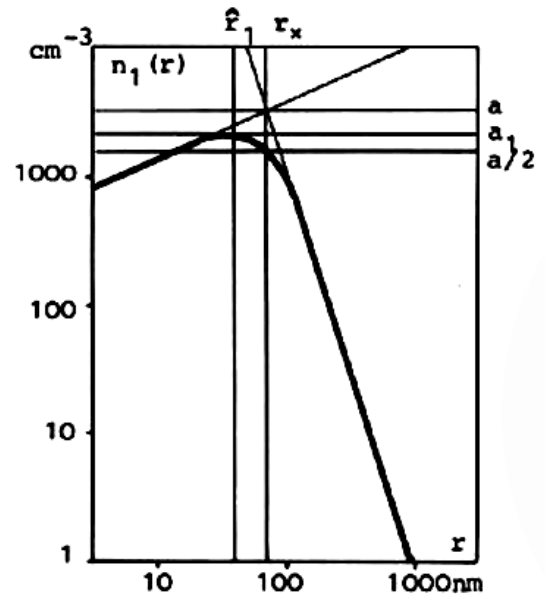
KL1 : $n_1(r) = a_1(k+1) / (l(r/\hat{r}_1)^k + k(\hat{r}_1/r)^l)$ - a modification of KLO, $\hat{r}_1 = (l/k)^{1/(k+1)} r_x$, $a_1 = a l^{1/(k+1)} k^{k/(k+1)} / (k+1)$. KLO is determined if $k+l > 0$, whereas KL1 is determined only if $k > 0$ and $l > 0$. Moment of the q -th order of the function $n_0(r) = n_1(r)/r$ exists if $-1 < q < k$ and is expressed by elementary functions

$$M_q = \int r^{q-1} n_1(r) dr = a \frac{r_x^q}{(k+1) \sin(\pi(1+q)/(k+1))} \quad (5)$$

the mode of the radius of the distribution $n_q(r) = r^{q-1} n_1(r)$ is

$$r_q = (l-1+q)/(k+1-q)^{1/(k+1)} r_x \quad (6)$$

Figure: KL-distribution. (r_x, a) - the intersection point of asymptotes, (\hat{r}_1, a_1) - the extremum of $n_1(r)$. k - the descent slope of the right asymptote, l - the ascent slope of the left asymptote. The figure depicts the best approximation to the distribution (4), $k = 3.15$, $l = 0.44$, $r_x = 72$ nm, $\hat{r}_1 = 42$ nm.



APPROXIMATION ERRORS

The mean square relative error of the approximation of the spectrum (4) in the interval $r = 5$ nm...5 μ m is 36% for S1 (S1A or S1B), 70% for S2 and 7% for KL. A thorough check-up of the accuracy of approximation has been carried out on the set of 271 empirical spectra registered by Mirme et al. in a two-week fair-weather period in summer 1986 at a rural site 50 km from a big city. The instrument described in [5] has been used. The values of the function $n_1(r)$ were approximated on the set of radii 5, 9, 16, 28, 50, 89, 158 nm. In MG and S1 the restrictions $\beta, s \geq 0.1$ were used. The procedure of approximation skipping the neighbourhood of zero converged to S1 in 1/3 of the cases and to MB in 2/3 of the cases. The results are presented in Table 1.

Table 1

Approximation errors of 271 spectra

Model	MG	S1	S2	KL
Average relative error	12%	16%	13%	8%
Maximum relative error	48%	40%	36%	18%
Frequency of turning out most adequate	22%	10%	19%	49%

LOSSES OF INFORMATION CAUSED BY NONORTHOGONALITY

Information losses and error amplification coefficients were determined in the neighbourhood of approximation of the spectrum (4). The matrix D was taken to be diagonal. Two variants $D_{ii} = \text{const}$ and $D_{ii} = \text{const} \cdot n_1^2(r)$ were considered. The calculations have been carried out on 13-point logarithmic set of radii from 5 nm to 5 μm . The results are presented in Table 2.

Table 2

Characteristics of models dependent on the nonorthogonality of the data-parameters transformation

At constant: Model	absolute errors						relative errors					
	SME	S1A	S1B	S2	KLO	KL1	SME	S1A	S1B	S2	KLO	KL1
ΔI : bit	12	20	4.3	10	3.2	2.0	8.9	13	4.0	4.7	3.2	2.2
ΔI : decimal digit	3.5	6.0	1.3	3.0	1.0	0.6	2.7	3.8	1.2	1.4	1.0	0.7
K	3.8	32	2.1	5.6	1.7	1.4	2.8	8.9	2.0	2.2	1.7	1.5

REFERENCES

1. Шифрин К.С. (1955) О вычислении радиационных свойств облаков. Труды ГГО, вып. 46, с. 5-33.
2. Смирнов В.И. (1973) Об аппроксимации эмпирических распределения по размерам облачных капель и других аэрозольных частиц. Изв. АН СССР, ФАО, т. 9, с. 54-65.
3. Smirnov V.I. (1984) On the mechanisms responsible for the formation of typical size spectra and vertical distribution tropospheric aerosol particles. In: Eleventh Int. Conf. Atmos. Aerosols, Cond. Ice Nuclei, Budapest, vol. 1, p. 82-86.
4. Смеркалов В.А. (1984) Аппроксимация среднего распределения аэрозольных частиц по размерам. Изв. АН СССР, ФАО, т. 20, с. 317-320.
5. Mirme A. et al. (1984) Multi-channel electric aerosol spectrometer. In: Eleventh Int. Conf. Atmos. Aerosols, Cond. Ice Nuclei, Budapest, vol. 2, p. 155-159.