Bull. Nov. Comp. Center, Num. Anal., 18 (2016), 49–56

On derivation of the size distribution of cloud droplets from the phase function*

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Abstract. This paper deals with an ill-posed problem to determine the size distribution for water drops in a cloud from a given scattering phase function. Numerical experiments have shown that a method based on non-negative least squares with additional requirements of smoothness can be used to solve the ill-posed problems.

Keywords: ill-posed problem, numerical method, scattering phase function, water drop clouds in the atmosphere, size distribution of water droplets.

1. Introduction and statement of the problem

This paper concerns a challenging problem of derivation of aerosol size distributions from phase function measurements, see, for example, [7, 15–17]. The optical properties of the atmospheric clouds can be described by the extinction cross-section, single scattering albedo and a phase function [11, 12]. These three characteristics depend on the light wavelength and the size distribution of particles in a cloud. The first two of them define the photon free path length and probability of scattering for a photon in a collision, while the phase function describes the distribution of the scattering angle (or its cosine). Under the assumption that the clouds consist of spherical water droplets, the optical characteristics can be computed by the Mie theory [1–3]. Examples of phase functions $g(\mu)$ for spherical water droplets for fixed sizes are presented in Figure 1. In this figure values of the scattering angle θ are presented on X-axes, $\mu = \cos\theta$, and $\int_{-1}^{1} g(\mu)\, d\mu = 1$.

Let us assume that the light wavelength is fixed, $g_r(\mu)$ is the phase function for water droplets of radius r, and $p(r)$ is the probability density of droplet radii in a cloud,

$$\int_{-1}^{1} g_r(\mu)\, d\mu = 1, \qquad \int_0^R p(r)\, dr = 1. \tag{1}$$

In this case the phase function $g(\mu)$ of the cloud is a superposition of the phase functions $g_r(\mu)$ for monodisperce media:

*Supported by the Russian Foundation for Basic Research under Grants 15-01-00783, 16-01-00145, by the Basic Research Program of the Presidium of the Russian Academy of Sciences (I.33), and by the Program "Leading Scientific Schools of Russia" (NSh-5111.2014.1).

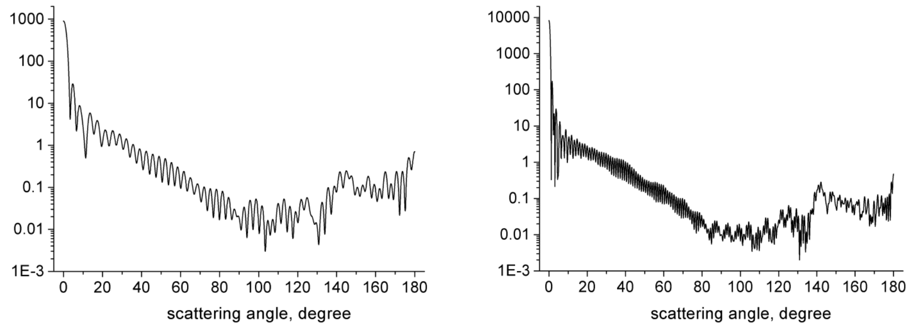

Figure 1. Scattering phase functions with wavelength 0.53 µm for a monodisperse medium containing water drops of radius 5 µm (left) and 15 µm (right)

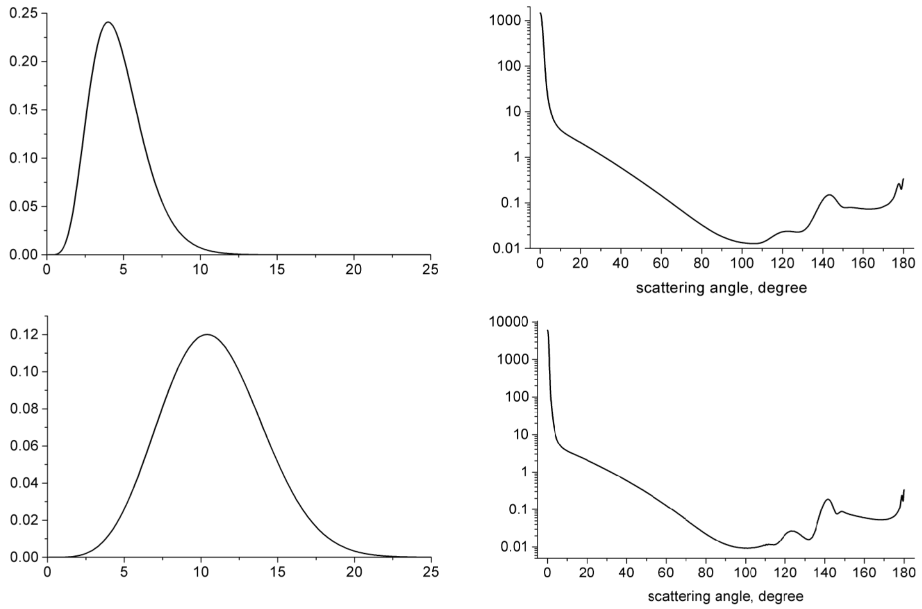

Figure 2. Probability densities (left) of the drop radius and scattering phase functions (right) with wavelength 0.53 µm for cloud models C1 (top) and OPAC Cumulus Maritime (bottom). Values of the cloud droplet radii are presented on X-axes in µm

$$g(\mu) = \int_0^R g_r(\mu) p(r)\, dr. \tag{2}$$

Examples of the probability density and the phase function for two cloud models are presented in Figure 2. For these models the droplets radii are distributed according to the modified gamma distribution:

$$p(r) = Cr^\alpha \exp(-Br^\gamma), \quad B = \frac{\alpha}{\gamma r_{\text{mod}}^\gamma},$$

where r is the radius of drops in µm, α, γ are the distribution parameters, and r_{mod} is the mode radius. The cloud model C1 [3] corresponds to

$$\alpha = 6, \quad \gamma = 1, \quad B = 1.5, \quad r_{\text{mod}} = 4,$$

and the OPAC Cumulus Maritime cloud model [6] has the following parameters

$$\alpha = 4, \quad \gamma = 2.34, \quad B = 0.00713, \quad r_{\text{mod}} = 10.3989.$$

Remark. The implementation of the Mie theory is nontrivial. In monograph [1] the author describes different approaches to numerically realize the Mie formulas for accurate computation of phase functions $g_r(\mu)$ for monodisperse media. Another problem is an accurate numerical integration according to formula (2). In order to obtain an appropriate result the integration step must be small enough. Figure 3 shows the result of inaccurate numerical integration for the OPAC Cumulus Maritime cloud model by the program "PolyMie" [13]. In this case, the step for integration by the trapezoidal rule is equal to $r_{\text{mod}}/50$ and R is defined by $p(R)/p(r_{\text{mod}}) \leq 0.005$. The program "Poly2" from [13] can be used for more exact calculations. In many cases thousands of summands are necessary for obtaining more or less precise results. The programs presented in [13] were developed in the Ludwig–Maximilian University of Munich on the basis of W. Wiscombe's code [19]. Additional modifications of these programs for more accurate and flexible computations were performed in the Institute of Computational Mathematics and Mathematical Geophysics SB RAS (Novosibirsk).

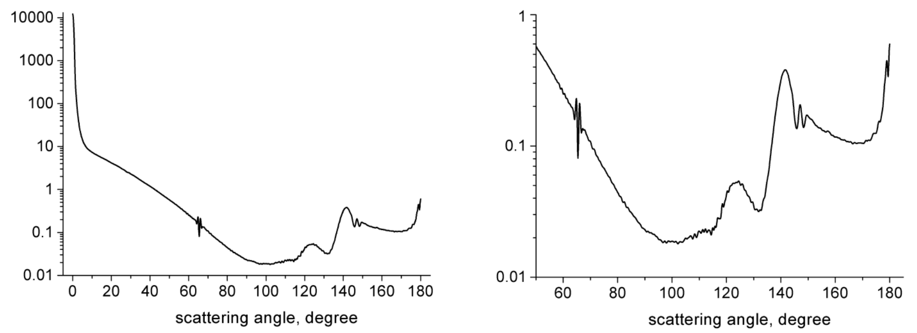

Figure 3. An example of inaccurate computation of the phase function for the OPAC Cumulus Maritime cloud model (see details in the text)

Assume now that the phase function is measured with some noise and we know the values b_i, $i = 1, \ldots, N$, which are the values of the scattering phase function of a cloud $g(\mu_i)$ at the points $\mu_i = \cos\theta_i$ with an additive noise:

$$b_i = g(\mu_i) + e_i, \quad \mu_i = \cos\theta_i, \quad i = 1, \ldots, N. \tag{3}$$

We want to estimate the probability density $p(r)$ of droplet radii in the cloud at the points r_j, $j = 1, \ldots, M$.

To solve this inverse problem, we use the following approximation for equation (2):

$$g(\mu) = \int_0^R g_r(\mu)p(r)\,dr = \sum_{j=1}^{M} \int_{S_j} g_r(\mu)p(r)\,dr \approx \sum_{j=1}^{M} p(r_j) \int_{S_j} g_r(\mu)\,dr. \tag{4}$$

Here $r_j \in S_j$, and S_j are the disjoint intervals of length $|S_j|$ such that $\bigcup_{j=1}^{M} S_j = (0, R)$. Moreover, we make a further (problematic) simplification:

$$\int_{S_j} g_r(\mu)\,dr \approx g_{r_j}(\mu)|S_j|,$$

and reduce the inverse problem to the following system of linear equations

$$Ax = b, \quad A = [A_{ij}], \tag{5}$$

where $b = (b_1, \ldots, b_N)^T$, $x = (p(r_1), \ldots, p(r_M))^T$, $A_{ij} = g_{r_j}(\mu_i)|S_j|$ for $i = 1, \ldots, N$, $j = 1, \ldots, M$.

The main objective is to find a vector x which approximately satisfies equation (5). In this case, the method of least squares fails. In the next section we will try the Tikhonov variational regularization to solve the ill-posed problem (see, for example, [8, 18]).

2. Numerical algorithm and results of computational experiments

We reduce the ill-posed problem to the minimization of the following functional

$$\|Ax - b\|^2 + \lambda \sum_{j=2}^{M-1} (x_{j+1} - 2x_j + x_{j-1})^2 \tag{6}$$

under additional constraints

$$x_j \geq 0, \quad \sum_{j=1}^{M} x_j|S_j| = 1. \tag{7}$$

The value λ is a parameter of the method. To solve problem (6), (7), we used a version of the reduced gradient method. Expressing $x_i > 0$ in terms of other variables from the equality constraint we arrive at the problem of minimizing the function of $M - 1$ variables provided non-negativity of the variables is respected. The Newton direction is obtained by using the modified Cholesky factorization of the Hessian [4]. To improve the numerical stability of the modified Cholesky factorization we applied symmetric permutations of the Hessian columns and rows.

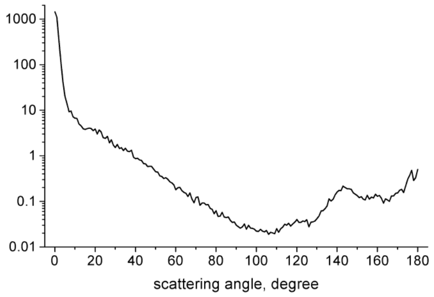

Figure 4

We have tested the performance of the approach (5)–(7) by computational experiments. The noise e_i in (3) was simulated by the formula

$$e_i = Cg(\mu_i)w_i, \quad i = 1, \ldots, N, \tag{8}$$

where w_i are independent standard Gaussian random variables. The value C will be called “noise intensity”, and we present it in percents. Figure 4 presents an example of the phase function for the cloud model C1 with noise intensity $C = 10\,\%$.

In Figures 5–7 we present results of the numerical experiments for the following parameters:

$$\begin{aligned} &i = 1, \ldots, N = 181, \quad \mu_i = \cos\theta_i, \quad \theta_i = (i-1)\pi/180, \\ &j = 1, \ldots, M = 25, \quad r_j = j \text{ µm}, \quad |S_j| = 1 \text{ µm}. \end{aligned}$$

We took the phase functions with additive noise (3), (8) as the right-hand side of equation (5). The noise intensity C is equal to $10\,\%$ in the numerical experiments with C1 cloud and the OPAC Cumulus Maritime model.

Figure 7 presents results for the bimodal probability density. Distributions of this type were considered for the cloud models in [9, 14]. The noise intensity C is equal to $5\,\%$ in this case. The table presents errors depending on the regularization parameter λ for this numerical experiment.

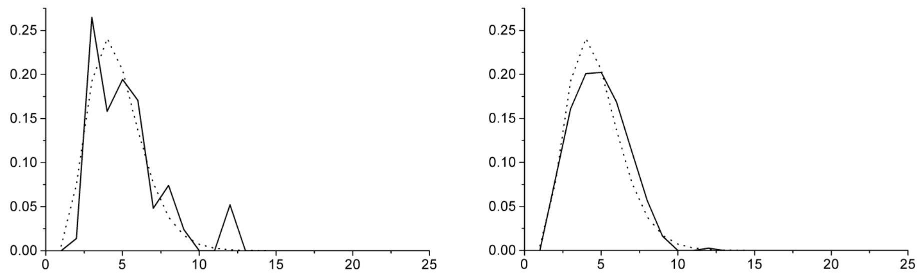

Figure 5. Numerical minimization of (6) under constraints (7) for $\lambda = 0$ (left) and $\lambda = 500$ (right). The probability density of the drop radius for the cloud model C1 is shown by dot lines, while the results obtained by the Tikhonov variational regularization are shown by solid lines

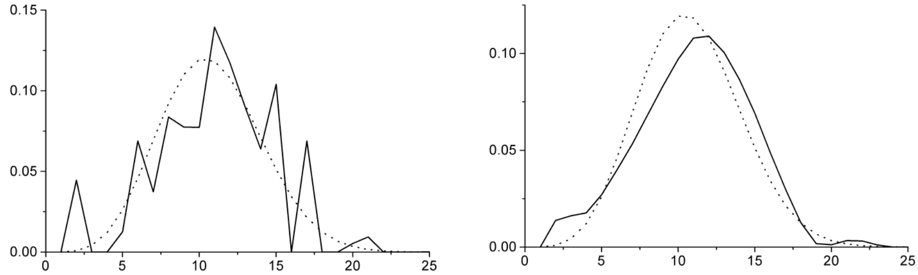

Figure 6. Numerical minimization of (6) under constraints (7) for $\lambda = 0$ (left) and $\lambda = 500$ (right). The probability density of the drop radius for the OPAC Cumulus Maritime model is shown by dot lines, while the results obtained by the Tikhonov variational regularization are shown by solid lines

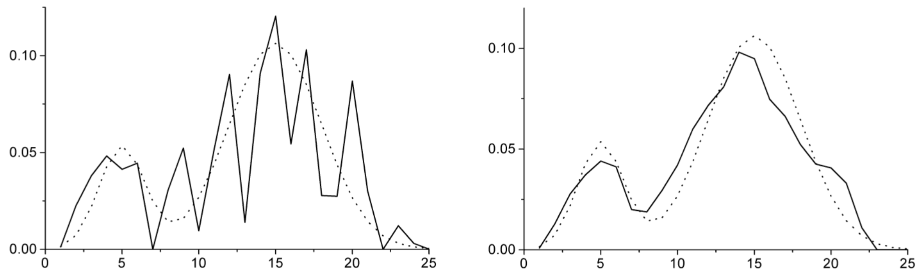

Figure 7. Numerical minimization of (6) under constraints (7) for $\lambda = 0$ (left) and $\lambda = 50$ (right). A bimodal probability density of the drop radius is shown by dot lines, while the results obtained by the Tikhonov variational regularization are shown by solid lines

Errors $\delta_1 = \sum_{j=1,\dots,M} |x_j - x_j^{\text{exact}}|$, $\delta_\infty = \max_{j=1,\dots,M} |x_j - x_j^{\text{exact}}|$ of the Tikhonov variational regularization method depending on the parameter λ for the bimodal probability density of the drop radius

λ	δ_∞	δ_1	λ	δ_∞	δ_1
0	0.0713	0.485	150	0.0221	0.234
10	0.0337	0.291	200	0.0231	0.236
50	0.0209	0.244	300	0.0247	0.242
100	0.0216	0.236	500	0.0272	0.259

Numerical experiments show that an appropriate approximation to the required probability densities can be found by the varying parameter λ. In the future we are planing to study several methods, like L-curve or GCV, to choose an appropriate value for the regularization parameter λ (see, for example, [5, 10]).

Acknowledgements. The authors would like to thank Prof. Ulrich G. Oppel and members of his research team for the cooperation, as well as Kim

Bazarov and Daria Mironova for their assistance in conducting numerical experiments.

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