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Analytical inversion of the absorption spectrum to determine non-spherical particle size distribution

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ABSTRACT

For a variety of non-spherical particles (oriented spheroids, cuboids, triangular prisms, and hexagonal prisms), analytical transform techniques are proposed to retrieve the particle size distribution (PSD) from measured absorption spectra. The absorption efficiency of particles is calculated using the anomalous diffraction theory (ADT). We find that for each type of non-spherical particles, there exists an ADT transform pair between the size distribution and the complex absorption spectrum, which provides the physical basis for solving the inverse problem. Furthermore, the relation between the size distribution and real absorption spectrum is established by using Gaver–Stehfest's method. The numerical calculations show that the use of extended precision instead of double precision arithmetic can produce more reliable results at the expense of computational efficiency. Also it is shown that a small Stehfest number (standing for truncation number) tends to enhance the anti-noise level of inversion.

1. Introduction

Atmospheric particles (aerosol and cloud droplets) can remarkably influence the Earth's radiation budget through scattering and absorbing solar and terrestrial radiation. In order to accurately understand and quantitatively calculate the radiative effect of atmospheric particles, a knowledge of particle size distribution (PSD) is generally required. In addition, retrieval of PSD will have broad application in many other areas such as biophysics, oceanophysics, and astrophysics.

The retrieval of PSD is a classic inversion problem. Over the past several decades, various inversion schemes have been applied to PSD of spherical particles. For example, there are regularization method [1–6], iterative method [7–10], computed tomography [11], genetic algorithm [12], moments method [13,14] and analytical method [4,15–20]. However, non-sphericity is one of the characteristics of aerosol and ice cloud particles, which restricts the applicability of the retrieval methods for designed spherical particles. Consequently, numerical methods to incorporate non-spherical scattering into the retrieval of PSD has become a subject of intensive research e.g., [21–35], although it requires large computational sources (such as CPU consumption and memory). Recently, an integral transform technique has been developed to retrieve PSD of non-spherical particles based on extinction spectrum

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[36–38]. In this method, the integral kernel function is expressed in a suitable closed-form by an approximate optical theory. Thus the PSD for various types of particle shape can be retrieved analytically. The main advantage of the integral transform technique lies in that it can significantly reduce the computing time providing a rapid result for an inversion problem.

All the existing inversion methods for PSD are primarily based on the measurement of light extinction and/or angular scattering. So far the inversion method for PSD based on the direct measurement of absorption has not been paid attention. This work provides a theoretical study for application of the integral transform technique for retrieval of PSD based on the input spectral absorption data. We believe that the presented new theory can enhance our knowledge for understanding the interaction between radiation and non-spherical particle. Also the proposed techniques can be used for some specific applications. In Section 2, the anomalous diffraction theory (hereafter ADT) [39] is introduced for absorption efficiency of particles. In Section 3, the formal solutions of non-spherical inversion problem are obtained in context of ADT for oriented spheroids, cuboids, triangular prisms, and hexagonal prisms. Also the ADT integral transform pairs are constructed for a variety of non-spherical particle shapes. Section 4 shows the real-variable inverse formulas for non-spherical particles. In Section 5, numerical simulations are accomplished to test the performance of the proposed method. In Section 6, we conclude with a brief discussion.

2. Inversion problem

For simplicity, it is assumed that the particulate system is made up of particles of same shape and varying sizes, and all particles have aligned orientations and the angle dispersion can be ignored. Then we can have the quantitative relationship between the polydisperse absorption coefficient and PSD by the Fredholm integral equation of the first kind

$$\beta_{abs}(k,m,\mu,\theta)=\int_0^\infty P(a,\mu,\theta)Q_{abs}(k,m,a,\mu,\theta)f(a)da, \tag{1}$$

where $f(a)$ is the PSD to be retrieved, $\beta_{abs}(k,m,\mu,\theta)$ is the measured absorption coefficient, k is the wavenumber of electromagnetic wave; $P(a,\mu,\theta)$ and $Q_{abs}(k,m,a,\mu,\theta)$ are the geometric cross section (projected area) and the absorption efficiency of a particle, which are shape and size dependent; $m=m_r+im_i$ is the complex refractive index of the particle relative to the medium with $m_i\geq 0$; a, μ and θ are the characteristic size, the nonsphericity and the orientation parameter of the considered particles, respectively. In Eq. (1), the integral equation reveals retrieval of $f(a)$ from the measured $\beta_{abs}(k,m,\mu,\theta)$ at a series of k.

The first requirement for analytical inversion is to find out an appropriate light scattering theory which can be used to build a closed-form expression of Q_{abs}. ADT is an approximation method which satisfies this requirement. However, the application of ADT conventionally requires that the index of refraction is close to unity and the particle size parameter is large enough. These constraints imply that the refraction and reflection are negligible as a ray passes through a particle. Thus the presence of particle will only produce change in the complex phase front of an incident plane wave over its geometrical shadowed area.

In ADT, the particle absorption efficiency is [39],

$$Q_{abs}=\frac{1}{P}\iint_P[1-\exp(-2\varphi_i)]dP, \tag{2}$$

where $\varphi_i=\mathrm{Im}(\varphi)$, Im indicates the imaginary part of a complex quantity, $\varphi=(m-1)k\Delta z$ is the local complex phase shift, Δz is a geometrical path length of a given ray through the considered particle. The integral is performed over the projected area P of the particle onto a plane perpendicular to the direction of light ray.

There exists a specific affine transformation relationship between extinction and absorption [39,40]. Thus the formula for absorption efficiency can also be inferred from the analytical result of extinction efficiency. Moreover, for a sufficiently small particle, it is easy to find that the integration of Eq. (2) is proportional to kV (where V is the volume of particle), which coincides precisely with the Rayleigh limit. Hence, we should emphasize that the ADT absorption formula can be applied not only to optically soft particles with large size but also to optically soft particles with arbitrary size.

Eq. (2) illustrates that the absorption by ADT is dependent on the particle shape and imaginary part of refractive index; the real part of refractive index has no contribution. This can simplify the mathematical treatment, but results in a loss of accuracy. The error for ADT absorption efficiency generally increases with $|m-1|$ increasing. For example, when $m=1.33+i0.01$, the maximum error can be up to 30% or even higher for spheres and cubes [41,42]. An effective way to improve the accuracy of ADT is through the inclusion of edge effect in absorption calculation [43]. However, this extra edge term can significantly enhance the difficulty of analytical inversion. Therefore the edge effect is not considered in this work.

3. Formal solutions and ADT transforms

PSD is assumed to satisfy the natural boundary conditions of $f(0)=0$ and $f(\infty)=0$, and $a^n f(a)$ is absolutely integrable for $n=\{0,1,2,3\}$.

The Laplace transform is a widely used mathematical tool for solving the inversion problems in physics and engineering. In a complex plane of κ, the Laplace transform to $a^n f(a)$ is

$$W_n(\kappa)=\int_0^\infty \exp(-\kappa a)[a^n f(a)]da, \tag{3}$$

and the inverse transform is

$$a^n f(a)=\frac{1}{2\pi i}\int_\gamma W_n(\kappa)\exp(\kappa a)d\kappa, \tag{4}$$

where the integral is usually taken along the so-called Bromwich contour γ running vertically from $\sigma-i\infty$ to $\sigma+i\infty$ for a real σ, and lying to the right of all the singularities of $W_n(\kappa)$.