OPTIMAL WAVELENGTH SELECTION ALGORITHM OF NON-SPHERICAL PARTICLE SIZE DISTRIBUTION BASED ON THE LIGHT EXTINCTION DATA

by

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Short paper
DOI: 10.2298/TSCI1205353T

In this paper, the anomalous diffraction approximation method is improved for calculating the extinction efficiency of non-spherical particles. Through this step, the range of the refractive index of particles can be enlarged, and the improved anomalous diffraction approximation method can be applied easily to the calculation of extinction efficiency for the most kinds of non-spherical particles. Meanwhile, an optimal wavelength selection algorithm is proposed for the inversion of non-spherical particle size distribution in the dependent mode. Through the improved anomalous diffraction approximation method, the computation time is substantially reduced compared with the rigorous methods, and a more accurate inversion result of particle size distribution is obtained using the optimal wavelength selection method.

Key words: *particle size distribution, light extinction, anomalous diffraction, wavelength*

Introduction

Atmospheric aerosols are suspensions of small solid or liquid particles in the atmosphere. To understand the effect of atmospheric aerosol on the atmospheric visibility degradation phenomena require knowledge of aerosol optical properties and their particle size distributions [1]. While particle size distribution is related to some processes such as nucleation [2], atomization [3], coagulation [4], deposition [5], synthesis [6], and breakage [7]. Light scattering particle sizing techniques have been widely used during the recent years since they provide an important tool for the characterization of a large number of industrial production processes. These techniques mostly contain the total light scattering, angle light scattering, diffraction light scattering and dynamic light scattering, and the measurement range of them ranges from nanometer to millimeter. It can in fact be used for on-line monitoring of micron or sub-micron particle systems thus providing real time measurements of both particle size distribution and particle concentration [8, 9]. But the calculation of extinction efficiency based on the classical Mie theory is complicated and time consuming, what is important is that the Mie theory can only be applied to the homogeneous spherical particle, while most particle systems are non-spherical particles. A suitable approximation method is the anomalous diffraction approximation (ADA), which can cal-

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culate the extinction efficiency of spherical and non-spherical particles [10-12]. Although some rigorous methods have been developed for calculating the extinction efficiency of randomly oriented non-spherical particle such as the extended boundary-condition method (T-matrix) and the finite-difference time-domain method (FDTD), the ADA is still an effective alternative which could avoid the complexity in calculating the extinction efficiency. In this paper, we will use the improved ADA method to calculate the extinction efficiency of non-spherical particles. Meanwhile, we will propose an optimal wavelength selection algorithm for the inversion of non-spherical particle size distribution in the dependent mode.

Theory and computation

When a beam of parallel monochromatic light passes through a particle system (thickness L) with its refractive index different from that of the dispersant medium, both the scattering and the absorption lead to an attenuation of the transmitted light. According to the Lambert-Beer law, the transmitted light intensity I is defined as $\ln I(\lambda)/I_0(\lambda) = -\tau(\lambda)L$ where $I_0(\lambda)$ is the incident light intensity at wavelength λ, $I(\lambda)/I_0(\lambda)$ is obtained by actual measurement, and $\tau(\lambda)$ is the turbidity.

In the absence of the multiple scattering and interaction effects, the transmitted light intensity I for a spherical particle system is given by the integral equation:

$$\ln\frac{I(\lambda)}{I_0(\lambda)} = -\frac{3}{2}LN_D\int_{D_{\min}}^{D_{\max}}\frac{Q_{ext}(\lambda,m,D)f(D)}{D}\,\mathrm{d}D \tag{1}$$

where $Q_{ext}(\lambda, m, D)$ is the extinction efficiency of a single spherical particle which is a function of the particle diameter D, the wavelength λ in the medium and the relative refractive index m can be calculated, N_D is the total number of particles, the lower and upper integration limits are denoted by $D_{\min}$ and $D_{\max}$, and $f(D)$ is the frequency distribution of a particle system. Within the framework of ADA, the extinction efficiency of a spheroidal particle has the same form as a sphere. When the incident light propagates along the rotation axis of the spheroidal particle, the extinction efficiency of a spheroidal particle is given by [14]:

$$Q_{ad} = 4\,\mathrm{Re}\left[\frac{1}{2} - i\frac{\exp(-iw)}{w} + \frac{1-\exp(-iw)}{w^2}\right] \tag{2}$$

where $w = 2ka(m - 1)/\lambda$, a is the semiaxis length of the rotation axis, and k – the wave number.

For a particle whose typical size is much larger than the incident wavelength or high absorbing, the edge can not be treated as sharp and the effect of the curvature by the particle must be included. After considering the edge effect term, the domain of applicability of ADA can be extended. The edge effect term is derived as: $Q_{edge}\ 2c_0a^{2/3}/k^{2/3}b^{4/3}$ where b is the semiaxis length of the other axis, $r = a/b$ is the aspect ratio, for prolate spheroid $r > 1$ and for oblate spheroid $r < 1$ and $c_0 = 0.996130$.

We use the standard ADA plus the edge term to calculate the extinction efficiency of spheroidal particles when the minor axis length is in the range from 1~10 μm, and the standard ADA is used when the minor axis length is in the range from 0.1~1 μm. According to the Lambert-Beer's law, the extinction caused by spheroidal particles with a particle size distribution $f(b, r)$ can be expressed as [15]:

$$\ln\frac{I(\lambda)}{I_0(\lambda)} = -LN_D \int_{b_{\min}}^{b_{\max}} \int_{r_{\min}}^{r_{\max}} Q_{ext}(\lambda, m, b, r) P(b, r) f(b, r) / V(b, r)\, \mathrm{d}b\, \mathrm{d}r \tag{3}$$

where Q_{ext} (λ, m, b, r) is the extinction efficiency of a spheroidal particle; here we use the angular averaging extinction efficiency. $P(b, r)$ is the averaging projected area of the particle, $f(b, r)$ – the frequency distribution function of particles in volume, and $V(b, r)$ – the volume of a spheroidal particle. The extinction values are calculated by the improve ADA method. The distribution of spheroidal particles is assumed to have R-R distribution with the expression:

$$f_{\text{R-R}}(b,r) = \left\{ \frac{k_b}{\overline{D}_b} \left(\frac{b}{\overline{D}_b} \right)^{k_b - 1} \exp\left[-\left(\frac{b}{\overline{D}_b} \right)^{k_b} \right] \right\} \left\{ \frac{k_r}{\overline{D}_r} \left(\frac{r}{\overline{D}_r} \right)^{k_r - 1} \exp\left[-\left(\frac{r}{\overline{D}_r} \right)^{k_r} \right] \right\} \tag{4}$$

where $\overline{D}_b$, k_b, $\overline{D}_r$, and k_r are the characteristic parameters of spheroidal R-R distribution. The visible extinction spectrums have relationship with the characteristic parameters of spheroidal R-R particle size distribution. If the visible extinction spectrum is a monotone ascending we have $\overline{D}_b < 1$ μm; $\overline{D}_b > 3.5$ μm for the visible extinction spectrum is a monotone descending; $\overline{D}_b > 2$ μm for the visible extinction spectrum is curving curve. When the relative refractive index of particles is fixed, the visible extinction spectrum are changed from a monotone ascending to curving and then to monotone descending with the increasing $\overline{D}_b$ (fig. 1).

We propose an optimal wavelength selection algorithm for the inversion of non-spherical particle size distribution in the dependent mode. The corresponding wavelengths were selected as the measurement wavelengths. Furthermore, the minimum and the maximal wavelengths in the visible region were also selected as the measurement wavelengths. Table 1 gives the inversion results of spheroidal particles with the proposed optimal wavelength selection algorithm. In tab. 1, No. 1 denotes that optimal wavelength selection algorithm is used and No. 2~No. 3 denote that wavelengths are selected with random methods. It is clear to see that good inversion results can be obtained with the optimal wavelength selection algorithm.

Table 1. Inversion results of spheroidal particles [($\overline{D}_b$, k_b, $\overline{D}_r$, k_r) = (3.5, 15, 1.5, 15)]

	(λ_1, λ_2, λ_3, λ_4, λ_5)/μm	Inversion results		Inversion error ς (0% random noise)
		0% random noise	1% random noise	
No. 1	(0.4, 0.46, 0.55, 0.65, 0.8)	(3.5004, 14.9815, 1.5024, 15.5709)	(3.4898, 14.0111, 1.4886, 17.8935)	$7.8007 \cdot 10^{-4}$
No. 2	(0.46, 0.55, 0.65, 0.7, 0.76)	(3.4998, 15.0781, 1.4880, 13.4745)	(3.4749, 14.0472, 1.4807, 13.3194)	0.0078
No. 3	(0.4, 0.5, 0.6, 0.7, 0.8)	(3.4998, 15.0546, 1.4926, 13.9040)	(3.4768, 16.1251, 1.4816, 13.1081)	0.0036
No. 4	(0.5, 0.53, 0.6, 0.7, 0.75)	(3.5006, 15.0744, 1.4838, 13.1063)	(3.5909, 16.0874, 1.4794, 17.3070)	0.0128

Conclusions

An improved ADA method is used for calculating the extinction efficiency of spheroidal particles, in which the complexity in calculating the extinction efficiency of non-sphe-

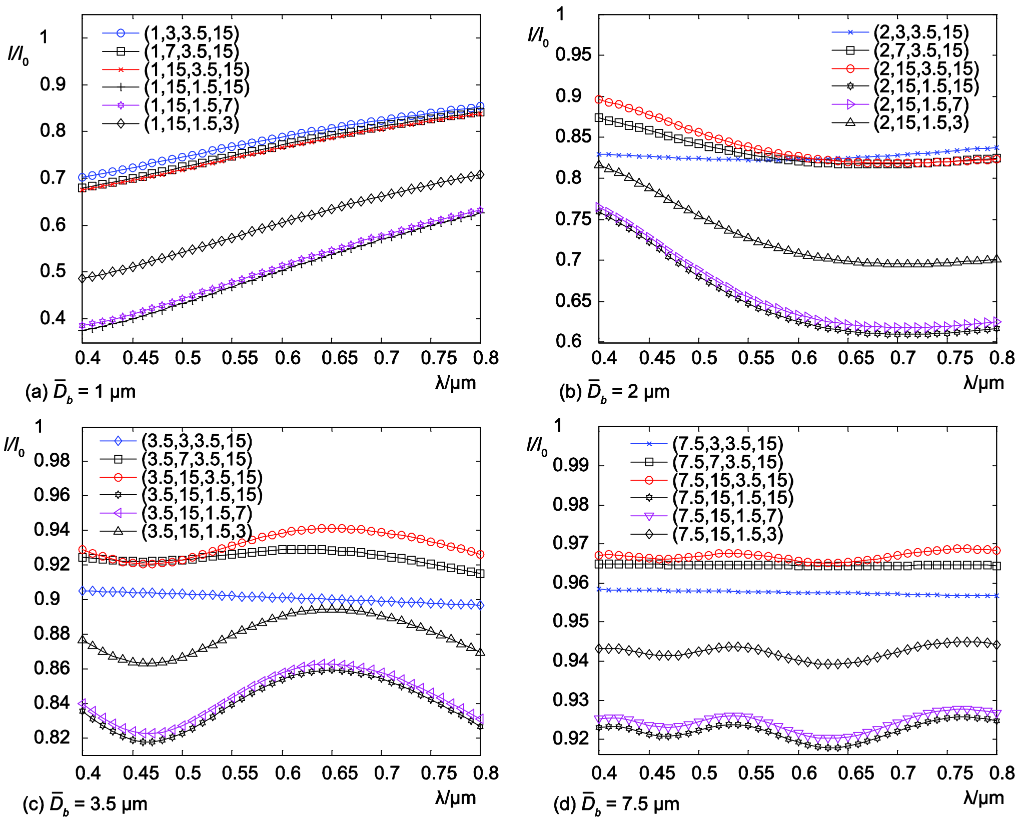

Figure 1. Visible extinction spectrums of spheroidal particles with R-R distributions (m = 1.235)

rical particles is diminished, and the computation time is substantially reduced. Meanwhile, the visible extinction spectrums of spheroidal particles are analyzed, and an optimal wavelength selection algorithm is proposed for the inversion of spheroidal particle size distribution. The visible extinction spectrums have relationship with the distribution of spheroidal particles, and the optimal wavelength selection algorithm can obtain good results for the inversion of spheroidal particle size distribution.

Acknowledgment

This work was supported by the National Natural Science Foundation of China (No. 11132008, No.11202202) and Zhejiang Province Natural Science Funds (Y6110147).

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Paper submitted: August 1, 2012
Paper revised: September 3, 2012
Paper accepted: September 12, 2012