INVERSION OF SPHEROID PARTICLE SIZE DISTRIBUTION IN WIDER SIZE RANGE AND ASPECT RATIO RANGE

by

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The non-spherical particle sizing is very important in the aerosol science, and it can be determined by the light extinction measurement. This paper studies the effect of relationship of the size range and aspect ratio range on the inversion of spheroid particle size distribution by the dependent mode algorithm. The T matrix method and the geometric optics approximation method are used to calculate the extinction efficiency of the spheroids with different size range and aspect ratio range, and the inversion of spheroid particle size distribution in these different ranges is conducted. Numerical simulation indicates that a fairly reasonable representation of the spheroid particle size distribution can be obtained when the size range and aspect ratio range are suitably chosen.

Key words: light extinction, spheroid, inversion, size range, aspect ratio range

Introduction

Atmospheric aerosols have an important effect in many atmospheric applications, and have some obvious influence on the Earth's radiation, cloud formation, and the air quality. A better understanding and explanation of the impact of atmospheric aerosol on the corresponding research field require the knowledge of the aerosol particle size distribution [1-3]. Moreover, the particle size distribution has important influence on the dynamic processes of particle systems, and it is very helpful to understand the dynamic evolution of particle size distribution [4-7].

Actually, there are some commonly used particle sizing methods, such as the light scattering measurement, light extinction measurement, as well as the remote sense measurement. Among these methods, the light extinction particle sizing measurement has been widely used since it can be measured by a simple optical layout and realized easily with only a few input parameters [8, 9].

In the light extinction measurement, the particle size distribution can be obtained by the inversion of the light extinction spectrum based on the Fredholm integral equation of the first kind. Because of the intrinsic ill-posedness of this integral equation, it has long been a subject of research to obtain a stable inversion result [10]. For the inversion algorithm of the light extinction measurement, there are classified into two algorithms: the dependent mode algorithm and the independent mode algorithm. In the dependent mode algorithm, much prior information is available and the true particle size distribution is inversed using a certain optimization algorithm. Since many particle systems often conform to some commonly used distribution function, the dependent mode algorithm is simpler and also used in this paper.

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In order to obtain the particle size distribution in the dependent mode algorithm with the light extinction measurement, the particle model should be assumed firstly. Usually, the spherical particle based on the Mie scattering theory is used to research the particle size distribution. Actually, most of particle systems are composed of the non-spherical particles that have the size distributions, shape distributions, and orientation distributions. Because the simplest non-spherical particle is the spheroid, understanding scattering by a spheroid should be helpful in the study on the scattering of the non-spherical particles [11]. Thus, we decide to use the spheroid to inverse the spheroid particle size distribution in the dependent mode algorithm based on the light extinction measurement. Meanwhile, the inversion of the spheroid particle size distribution is conducted with different size range and aspect ratio range. In doing so, we can obtain the relationship of the size range and aspect ratio range with the inversion results, and then we can achieve good representation for the inversion of the spheroid particle size distribution with the light extinction measurement.

Method and computation

In the particle sizing for the spheroid particles with the light extinction measurement, the spheroid particle needs two characteristic parameters to describe the particle size: *b* is the maximum radius perpendicular to the main symmetry axis, ε is the aspect ratio (ratio of *a/b*, *a* denotes the radius of the spheroid along its main symmetry axis, for a prolate spheroid $\varepsilon > 1$, for an oblate spheroid $\varepsilon < 1$).

According to the Lambert-Beer law, the light extinction of an ensemble of spheroid particles is represented by the Fredholm integral equation of the first kind [12, 13]:

$$\ln \frac{I(\lambda_i)}{I_0(\lambda_i)} = -LN \int_{\varepsilon_{\min}}^{\varepsilon_{\max}} \int_{b_{\min}}^{b_{\max}} C_{\text{ext}}(\lambda_i, m, \varepsilon, b) f(\varepsilon, b) d\varepsilon db$$
(1)

where $I_0(\lambda_i)$ is the incident light intensity at wavelength, $I(\lambda_i)$ – the transmitted light intensity, C_{ext} – the extinction cross-section of a spheroid particle, m – the relative complex refractive index (the ratio between the particle and medium refractive index), L – the length of the particle system, N – the total spheroid particle number per unit volume, and $f(\varepsilon, b)$ – the unknown spheroid particle size distribution.

For simplicity, we assume the distributions f(b) and $f(\varepsilon)$ are independent. That is to say eq. (1) can be rewritten [14]:

$$\ln \frac{I(\lambda_i)}{I_0(\lambda_i)} = -LN \int_{\varepsilon_{\min}}^{\varepsilon_{\max}} f(\varepsilon) d\varepsilon \int_{b_{\min}}^{b_{\max}} C_{\text{ext}}(\lambda_i, m, \varepsilon, b) f(b) db$$
(2)

In the inversion of the spheroid particle size distribution, the extinction cross-section of a spheroid particle C_{ext} should be calculated firstly. Among the calculating methods for the extinction cross-section of spheroids, the T matrix method is the fastest and the most powerful calculating method for the rigorously computing of the light scattering for the spheroids. However, the T matrix method has the limitation of the converged range, and it can be applied to calculate the light scattering of spheroids with small and moderate sizes [15]. It is obvious that the maximal convergent size parameters strongly depend on the size parameter, refractive index and the asphericity, especially for the case that when the particles become more aspherical. On the other hand, the geometric optical method (GOM) is an approximation method that can calculate the light scattering of spheroid particles at enough large size regions. In order to decrease the lower limit of this approximated method, the improved geometric optical method (IGOM) developed by Yang and Liou is applied to calculate the extinction cross-section of spheroids with larger sizes [16]. That is to say the T matrix method is used to calculate the extinction cross-section of spheroids for small and moderate sizes until the T matrix convergence is achieved. After that, the IGOM is used to continue to calculate the extinction cross-section of spheroids at large size. Through this combination, we can calculate the extinction cross-section of spheroids with wider size range and aspect ratio range.

For the dependent mode algorithm, the distribution function form should be assumed beforehand. After that the characteristic parameters of distributions f(b) and f(c) can be obtained by an optimal algorithm, and then the spheroid particle size distribution is inversed according to these characteristic parameters of the assumed distribution functions.

Generally, f(b) is assumed to have the log normal distribution, eq. (3), Rosin-Rammler (R-R) distribution, eq.(4). $f(\varepsilon)$ also has been assumed to be the equip probable distribution, eq. (5), or has the same distribution as f(b) [13]:

$$f(b) = \frac{1}{\sqrt{2\pi}\ln\sigma b} \exp\left[-\frac{1}{2}\left(\frac{\ln b - \ln u}{\ln\sigma}\right)^2\right]$$
(3)

where u and σ are the characteristic parameters of log normal distribution,

$$f(b) = \frac{k}{\overline{b}} \left(\frac{b}{\overline{b}} \right)^{k-1} \exp\left[-\left(\frac{b}{\overline{b}} \right)^k \right]$$
(4)

where k and \overline{b} are the characteristic parameters of R-R distribution, and

$$f(\varepsilon) = \frac{1}{\varepsilon_2 - \varepsilon_1}, \qquad \varepsilon_1 \le \varepsilon \le \varepsilon_2 \tag{5}$$

where ε_1 and ε_2 are the minimum and the maximum.

Table 1 lists the inversion results of spheroid particle size distribution with different size range and aspect range. It should be noted that the units of *b* is μ m, and ε is dimensionless. The true f(b) is assumed to be log normal distribution with $(u_b, \sigma_b) = (0.8, 1.3)$ in the range from 0.1 to 3 in step of 0.04, and the true $f(\varepsilon)$ is assumed to be log normal distribution with $(u_{\varepsilon}, \sigma_{\varepsilon}) = (1.2, 1.2)$ in the range from 1/3 to 3. For the inversion of this particle system, we use the genetic algorithm as the optimal method to obtain the characteristic parameters. From tab. 1, it is clear to see that good inversion results can be obtained with the same size

Table 1. Inversion of spheroid particle size distribution. f(b) is assumed to be log normal, $0.1 \le b \le 3$, $f(\varepsilon)$ is assumed to be log normal, $1/3 \le \varepsilon \le 3$, their characteristic parameters are $(u_b, \sigma_b, u_{\varepsilon}, \sigma_{\varepsilon}) = (0.8, 1.3, 1.2, 1.2), m = 1.3$

| Inversion | b: 0.1:0.04:3 | b: 0.1:0.1:10 | b: 0.1:0.04:3 | b: 0.1:0.1:10 |
|---------------|-----------------------------|---------------------------------|---------------------------------|-----------------------------|
| range | $1/3 \le \varepsilon \le 3$ | $1/2.4 \le \varepsilon \le 2.4$ | $1/2.4 \le \varepsilon \le 2.4$ | $1/3 \le \varepsilon \le 3$ |
| Inversion | (1.2, 1.2, | (1.019, 1.788, | (1.193, 1.201, | (1.07, 1.872, |
| results | 1.283, 0.783) | 1.031, 2.949) | 1.465, 0.962) | 1.161, 2.905) |
| Error | 1.7260e-4 | 0.3654 | 3.6264e-4 | 0.1520 |
| Inversion | (1.133,1.215, | (1.539, 1.686, | (1.207, 1.189, | (1.078, 1.892, |
| results (±1%) | 1.508, 1.425) | 1.814, 1.998) | 1.767, 1.399) | 1.159, 2.869) |
| Error (±1%) | 0.1320 | 1.5217 | 0.2436 | 0.0851 |

range and aspect ratio range as that in the true distribution, and if the inversion size range and aspect ratio range are different from the true range, the inversion results may produce large errors when 0% random error is added into the incident and transmitted light intensity. On the other hand, when $\pm 1\%$ random error is added into the incident and transmitted light intensity, the inversion results with larger size range and aspect ratio range as that in the true distribution. However, poor inversion results can be obtained with smaller aspect ratio range even the size range is the same as the true size range. So the aspect ratio range has obvious effect for the inversion of the spheroid particle size distribution.

Table 2 lists the inversion results of spheroid particle size distribution with different size range and aspect range. The true f(b) is assumed to be log normal distribution with $(u_b, \sigma_b) = (2, 1.1)$ in the range from 0.1 to 10 in step of 0.1, and the true $f(\varepsilon)$ is assumed to be log normal distribution with $(u_c, \sigma_{\varepsilon}) = (1.3, 1.3)$ in the range from 1/2.4 to 2.4. In tab. 2, we can see that the inversion results with wider size range and wider aspect ratio range are as good as those with the true size range and aspect range when 0% or ±1% random noise is added. Whereas, the inversed spheroid particle size distribution is badly constructed with smaller size range even in the case that the wider aspect ratio range is applied at the same condition.

| Inversion | b: 0.1:0.04:3 | <i>b</i> : 0.1:0.1:10 | <i>b</i> : 0.1:0.04:3 $1/2.4 \le \varepsilon \le 2.4$ | b: 0.1:0.1:10 |
|---------------|-----------------------------|---------------------------------|---|-----------------------------|
| range | $1/3 \le \varepsilon \le 3$ | $1/2.4 \le \varepsilon \le 2.4$ | | $1/3 \le \varepsilon \le 3$ |
| Inversion | (1.084, 1.998, | (1.099, 1.2, | (1.089, 2, | (1.098, 2, |
| results | 1.371, 1.325) | 1.3, 1.299) | 1.363, 1.313) | 1.301, 1.308) |
| Error | 0.0025 | 1.2746e-6 | 1.6783e-4 | 1.2759e-4 |
| Inversion | (1.012, 1.996, | (1.676, 1.559, | (1.064, 1.997, | (1.751, 1.482, |
| results (±1%) | 2.118, 2.345) | 1.425, 0.978) | 1.399, 1.452) | 1.822, 1.23) |
| Error (±1%) | 1.1288 | 0.3126 | 0.6604 | 0.3840 |

Table 2. Inversion of spheroid particle size distribution; f(b) is assumed to be log normal, $0.1 \le b \le 10$, $f(\varepsilon)$ is assumed to be log normal, $1/2.4 \le \varepsilon \le 2.4$, their characteristic parameters are $(u_{br}\sigma_{br}u_{er}\sigma_{c}) = (2.0,1.1,1.3,1.3), m = 1.3.$

Figure 1 shows the inversion results of the spheroid particle size distribution. The true f(b) is assumed to be R-R with characteristic parameter $(\bar{b}_b, k_b) = (1.2, 8)$ in the size range $0.1 \le b \le 10$ in step of 0.1. $f(\varepsilon)$ is assumed to be R-R with characteristic parameter $(\bar{b}_{\varepsilon}, k_{\varepsilon}) = (0.5, 5)$ in the aspect ratio range from $1/3 \le \varepsilon \le 3$. In this test, no noise is added and the inversion is conducted with different size range and aspect ratio range. As shown in figure 1, the inversion with the same wider size range and aspect ratio range is better than other inversion results. Table 3 is the same as in figure 1 but with $\pm 1\%$ random noise. We can see that inversion result with the smaller size range and smaller aspect ratio range produce large errors corresponding to those with the wider size range and wider aspect ratio range.

Table 3. Inversion of spheroid particle size distribution with $\pm 1\%$ random noise. f(b) is assumed to be R-R, $0.1 \le b \le 10$, $f(\varepsilon)$ is assumed to be R-R, $1/3 \le \varepsilon \le 3$, their characteristic parameters are $(\overline{b}_b, k_b, \overline{b}_s, k_c) = (1.2, 8, 0.5, 5)$, m = 1.3

| Inversion range | b: 0.1: 0.04: 3 $1/3 \le \varepsilon \le 3$ | b: 0.1:0.1:10 $1/2.4 \le \varepsilon \le 2.4$ | <i>b</i> : 0.1:0.04:3 $1/2.4 \le \varepsilon \le 2.4$ | b: 0.1:0.1:10 $1/3 \le \varepsilon \le 3$ |
|----------------------|--|--|---|--|
| Inversion results | (8.644, 1.211, 2.005, 0.597) | (11.811, 1.185, 2.221, 0.396) | (14.515, 1.189, 2.402, 0.403) | (14.531, 1.195, 1.09, 0.464) |
| Error | 0.1435 | 0.1318 | 0.2262 | 0.1294 |





Figure 1. Inversion of spheroid particle size distribution with no noise; f(b) is assumed to be R-R, 0.1 $\leq b \leq 10$, $f(\varepsilon)$ is assumed to be R-R, $1/3 \leq \varepsilon \leq 3$, their characteristic parameters are $(\bar{b}_b, k_b, \bar{b}_s, k_c) = (1.2, 8, 0.5, 5)$, m = 1.3; (a) true distribution, (b) inversion result with $0.1 \leq b \leq 10$, $1/2.4 \leq \varepsilon \leq 2.4$. (c) inversion result with $0.1 \leq b \leq 10$, $1/3 \leq \varepsilon \leq 3$, (d) inversion distribution with $0.1 \leq b \leq 3$, $1/3 \leq \varepsilon \leq 3$ (for color image see journal web site)

Figure 2 shows the inversion results of spheroid particle size distribution with different size range and aspect ratio range. The true f(b) is assumed to be R-R with characteristic parameter $(\bar{b}_b, k_b) = (1.2, 8)$ in the range from 0.1 to 3 in step of 0.04. $f(\varepsilon)$ is assumed to be equi-probable distribution in the range from $1/3 \le \varepsilon \le 3$. Since the distribution $f(\varepsilon)$ is known once the aspect ratio range is determined if the $f(\varepsilon)$ is assumed to be the equi-probable distribution. So there are two characteristic parameters unknown for this particle system. In figure 2, case 1 is $0.1 \le b \le 3$, $1/3 \le \varepsilon \le 3$, case 2 is $0.1 \le b \le 3$, $1/2.4 \le \varepsilon \le 2.4$, case 3 is $0.1 \le b \le 10$, $1/3 \le \varepsilon \le 3$, and case 4 is $0.1 \le b \le 10$, $1/2.4 \le \varepsilon \le 2.4$. It is obvious that completely reliable inversion results can be obtained for case 1 and case 3, whereas less accurate results may be produced for case 2 and case 4, which suggests the aspect ratio range is very important for the inversion of spheroid particle size distribution. If we want to achieve better representation of the true distribution, the aspect ratio should be applied with wider range.

Figure 3 shows the inversion results of spheroid particle size distribution with different size range and aspect ratio range. The true f(b) is assumed to be R-R with characteristic



Figure 2. Inversion of spheroid particle size distribution; f(b) is assumed to be R-R, $0.1 \le b \le 3$ with characteristic parameter $(\overline{b}_b, k_b) = (1.2, 8), f(\varepsilon)$ is assumed to be equi-probable distribution, $1/3 \le \varepsilon \le 3$, m = 1.3; (a) 0% noise, (b) ±1% noise (for color image see journal web site)



Figure 3. Inversion of spheroid particle size distribution, f(b) is assumed to be R-R, $0.1 \le b \le 3$, $f(\varepsilon)$ is assumed to be R-R, $1/3 \le \varepsilon \le 3$, their characteristic parameters are $(\overline{b}_b, k_b, \overline{b}_s, k_{\varepsilon}) = (2, 7, 1.5, 10)$, m = 1.3; (a) 0% noise, (b) ±1% noise (for color image see journal web site)

parameter (b_b , k_b) = (1.2, 8) in the range from 0.1 to 3 in step of 0.04. $f(\varepsilon)$ is assumed to be R-R distribution in the range from $1/3 \le \varepsilon \le 3$. However, we decide to inverse this distribution by assuming $f(\varepsilon)$ is the equi-probable distribution. It can be seen clearly that the inversion results with case 1 and case 3 are still acceptable even is $\pm 1\%$ random noise added. Thus, if the aspect ratio distribution is not known specifically, we can assume it to be the equi-probable distribution, and then inverse the size distribution using wider size range and aspect ratio range.

Table 4 lists the inversion results of spheroid particle size distribution with different size range and aspect ratio range. The true f(b) is the log normal with $(u_b, \sigma_b) = (1.2, 1.2)$ from 0.1 to10, and $f(\varepsilon)$ is also the log normal with $(u_{\varepsilon}, \sigma_{\varepsilon}) = (0.8, 1.3)$ from 1/2.4 to 2.4. When obtaining the spheroid particle size distribution with the dependent mode inversion method, $f(\varepsilon)$ is assumed to be the equi-probable distribution with two different aspect ratio range. It is ob-

Table 4. Inversion of spheroid particle size distribution; f(b) is assumed to be log normal, $0.1 \le b \le 10$, $f(\varepsilon)$ is assumed to be log normal, $1/2.4 \le \varepsilon \le 2.4$, their characteristic parameters are $(u_b, \sigma_b, u_{\varepsilon}, \sigma_{\varepsilon}) = (1.2, 1.2, 0.8, 1.3), m = 1.3$

| Inversion range | b: 0.1:0.04:3 $1/3 \le \varepsilon \le 3$ | b: 0.1:0.1:10 $1/2.4 \le \varepsilon \le 2.4$ | <i>b</i> : 0.1:0.04:3 $1/2.4 \le \varepsilon \le 2.4$ | b: 0.1:0.1:10 $1/3 \le \varepsilon \le 3$ |
|----------------------------|--|--|---|--|
| Inversion results | (1.377, 1.061) | (1.201, 1.164) | (1.201, 1.165) | (1.212, 1.173) |
| Inversion results (±1%) | (1.374, 1.054) | (1.191, 1.167) | (1.171, 1.181) | (1.491, 1.126) |

vious that the inversion result of f(b) using the assumed equi-probable distribution as the $f(\varepsilon)$ with the wider size range and aspect ratio range is closed to the true f(b).

According to all the simulations mentioned, we can come to a conclusion. That is the size range especially the aspect ratio range has strong effect on the inversion of spheroid particle size distribution in the dependent mode algorithm based on the light extinction measurement. Larger size range and aspect range should be used if good inversion results of the spheroid particle size distribution needed to be obtained. It should be noted that the inversion results still are satisfactory with the wider size range and aspect range when using the equiprobable aspect ratio distribution, even the assumed aspect ratio distribution $f(\varepsilon)$ do not conform with the true distribution.

Conclusions

In this paper, the light scattering and the inversion of spheroid particle size distribution in the dependent mode algorithm based on the light extinction technique are studied. For the extinction efficiency of spheroids, we use the T matrix to calculate the small and moderate particles, and at the same time the IGOM is applied for the large particles. Through this combination, the extinction efficiency of spheroids can be obtained in the wider size range and wider aspect ratio range. After that, the inversion of spheroid particle size distribution in the dependent mode algorithm is conducted with different size range and aspect ratio range, which indicates that the size range and aspect range of spheroids have obvious effect on the inversion of spheroid particle size distribution. Wider size range, especially the aspect range of spheroids should be considered. What is more important is that acceptable inversion results can be obtained with larger size range and aspect ratio range if the $f(\varepsilon)$ is assumed to be the equi-probable aspect ratio which is not known beforehand. So this research is very important, and it is very help for the inversion of the spheroid and non-spherical particle size distributions.

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