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Indetermination of particle sizing by laser diffraction in the anomalous size ranges

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ABSTRACT

The laser diffraction method is widely used to measure particle size distributions. It is generally accepted that the scattering angle becomes smaller and the angles to the location of the main peak of scattered energy distributions in laser diffraction instruments shift to smaller values with increasing particle size. This specific principle forms the foundation of the laser diffraction method. However, this principle is not entirely correct for non-absorbing particles in certain size ranges and these particle size ranges are called anomalous size ranges. Here, we derive the analytical formulae for the bounds of the anomalous size ranges and discuss the influence of the width of the size segments on the signature of the Mie scattering kernel. This anomalous signature of the Mie scattering kernel will result in an indetermination of the particle size distribution when measured by laser diffraction instruments in the anomalous size ranges. By using the singular-value decomposition method we interpret the mechanism of occurrence of this indetermination in detail and then validate its existence by using inversion simulations.

1. Introduction

Laser diffraction is one of the most popular methods of characterizing particles by measuring the light they scatter. Measurements executed according to this method are fast, nonintrusive, reliable, and are widely used in spray and solid particle diagnostics. The light scattered by a single spherical particle can be strictly described by the Mie theory, which is based on Maxwell's equations [1]. Instruments based on this method are called laser diffraction instruments. In laser diffraction instruments, the intensity of the scattered light of particles is usually obtained by accumulating a series of discrete photoelectric detections and the integration on the detections leads to a scattered energy distribution (SED). The particle size distribution (PSD) can be inverted from the measured SED. Although it has been around 50 years since the appearance of the first laser diffraction instrument, the traditional understanding of the basic scattering laws of particles is not entirely correct. It is reported that the angles to the location of the main peak of SEDs shift to large values and the Airy disk size of non-absorbing spherical particles becomes larger with increasing particle size in certain size ranges and these phenomena are called anomalous change of scattered energy distribution(ACSED) and anomalous change of Airy disk (ACAD) respectively [2,3]. In literature [3], it is proved that ACAD is caused by the interference of the diffracted light and the refracted light; therefore, it only exists for non-absorbing particles and weakly absorbing particles. Moreover, the analytical formulae for the bounds of the size ranges where ACAD occurs are also derived and the laws of ACAD are obtained in literature [3].

One may infer that ACSED and ACAD are caused by the same reason, although literature [2] points out the influence of ACSED on particle size analysis through concrete examples, it lacks universal arguments. In this paper, we mainly investigate the laws of ACSED and its influence on the Mie scattering kernel. Then, by using the singular-value decomposition (SVD) method, we interpret how this anomalous signature of the Mie scattering kernel influences the inverse procedure. Then, through inversion simulations of the forward directions, we validate the existence of the indetermination of particle sizing in the anomalous size ranges.

2. Principle of the laser diffraction method

A typical set-up for a laser diffraction instrument is given in Fig. 1. An expanded laser source illuminates particles in the measuring zone and the scattered light is measured by detectors at the focal plane of the Fourier lens. The scattering data is converted to electrical signals and transmitted to a computer and the PSD is then obtained after data processing. The energy ***E*** scattered by

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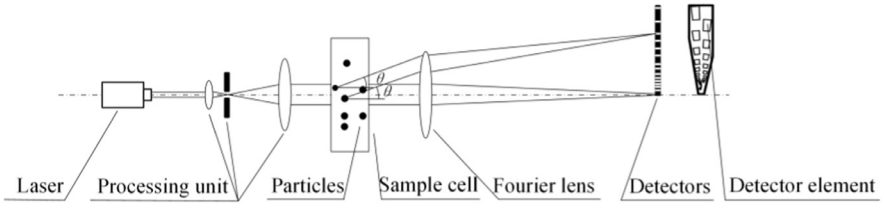

Fig. 1. A typical set-up for a laser diffraction instrument.

a single particle measured by a detector element with an average scattering angle of θ_i and an area of Δs_i can be expressed as

$$E(\theta_i, \alpha, m) = \iint_{\Delta s_i} I(\theta, \alpha, m) ds, \tag{1}$$

where θ is the scattering angle, $\alpha = \pi\ d\ /\ \lambda$ is the size parameter (d is the diameter of the particle, λ is the wavelength of light in the dispersion medium), $m = m_1\ /\ m_2$ is the refractive index of the particle relative to the dispersion medium, and $I\ (\theta,\ \alpha,\ m)$ stands for the intensity of the scattered light. When the integral interval is small, the scattered intensity is approximately linear with the changing of the scattering angle. Eq. (1) can be written as

$$E(\theta_i, \alpha, m) \approx I(\theta_i, \alpha, m)\Delta s_i. \tag{2}$$

In the ideal design for a laser diffraction instrument, the area of a detector element increases linearly with the average scattering angle, namely,

$$\Delta s_i = C\theta_i. \tag{3}$$

Here, C is a constant and can be neglected due to the inverse procedure, where we only need the relative SED. Assuming that the detector elements are continuous and, therefore, the range of the scattering angle corresponding to each element is sufficiently small, we can rewrite Eq. (2) by substituting Eq. (3) as

$$E(\theta, \alpha, m) = I(\theta, \alpha, m)\theta. \tag{4}$$

In actual laser diffraction instruments, for a PSD with a volume frequency of $W\ (\alpha)$, the number of particles in the area range $\alpha \to \alpha + d\alpha$ is directly proportional to $W\ (\alpha)\ d\alpha\ /\ \alpha^3$. According to Eq. (1), the scattered energy measured by the ith detector element can be described as

$$E'(\theta_i, m) = \int E(\theta_i, \alpha, m)\frac{W(\alpha)}{\alpha^3}d\alpha = \int \frac{W(\alpha)}{\alpha^3}\iint_{\Delta s_i} I(\theta, \alpha, m) ds d\alpha. \tag{5}$$

The continuous size range is divided into a series of discrete size segments: $\alpha_0 \to \alpha_1$, $\alpha_1 \to \alpha_2$, ..., $\alpha_{j-1} \to \alpha_j$, ..., $\alpha_{N-1} \to \alpha_N$, where N is the number of size segments. The volume frequency of the jth size segment is denoted as W_j and applying this to Eq. (5), $E'\ (\theta_i,\ m)$ can be denoted as E_i and Eq. (5) can be rewritten as

$$E_i = K_{i,j}W_j. \tag{6}$$

The Mie scattering kernel $\boldsymbol{K}$ can be described as

$$K_{i,j} = \frac{1}{\alpha_j - \alpha_{j-1}}\int_{\alpha_{j-1}}^{\alpha_j}\frac{1}{\alpha^3}\iint_{\Delta s_i} I(\theta, \alpha, m) ds d\alpha. \tag{7}$$

Obviously, Eq. (6) is formulated in terms of a Fredholm integral equation of the first kind. Owing to the ill-posedness and strong ill-conditioning of Eq. (6), the direct solution is unstable and unrealistic. Until now, there are plenty of publications focused on solving Eq. (6) and a number of algorithms are proposed, such as the Twomey method [4], Projection algorithm [5], Chahine algorithm [6–8] and Inverse Monte Carlo method [9]. These algorithms are mainly based on the following criteria,

$$\begin{cases} \sum_{i=1}^{M}\left(K_{i,j}W_j - E_i\right)^2 = \min \\ W_j \geq 0 \end{cases}, \tag{8}$$

where M is the number of detector elements and W_j is non-negative to make the solutions meaningful. Because of the ill-posedness of this inverse problem, there are multiple solutions satisfying Eq. (8), most of the solutions may have unrealistic, high frequency oscillations [10]. To avoid these high frequency oscillations, most algorithms apply smoothness criteria in the inverse procedure [11].

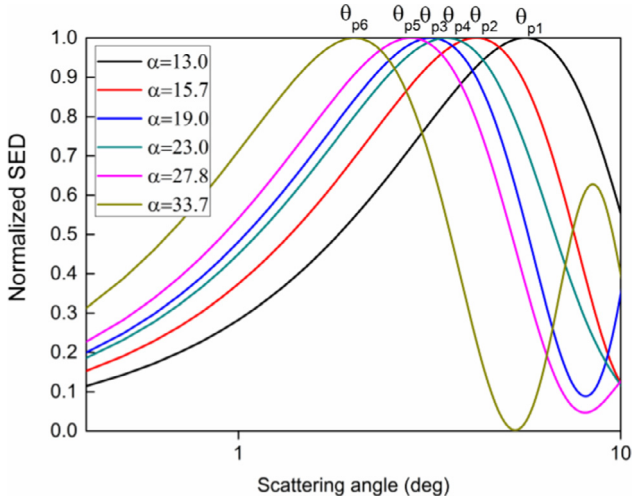

Fig. 2. SEDs of $\alpha = 13.0$, 15.7, 19.0, 23.0, 27.8, and 33.7 obtained by using the Mie theory for $m = 1.2$.

3. Anomalous change of the SEDs

The Mie scattering kernel is directly related to the inverted PSD; therefore, it is necessary to analyze the signature of the Mie scattering kernel. Although the scattered intensity $I\ (\theta,\ \alpha,\ m)$ decreases gradually with increasing scattering angle, the first peak (hereinafter referred to as the main peak) of the SED is located at a certain scattering angle θ_p. Fig. 2 shows the SEDs of $\alpha = 13.0$, 15.7, 19.0, 23.0, 27.8, and 33.7 obtained by using the Mie theory for $m = 1.2$. The angles to the location of the main peaks are denoted as θ_{p1}, θ_{p2}, θ_{p3}, θ_{p4}, θ_{p5}, and θ_{p6}, and the values are 5.59°, 4.17°, 3.19°, 3.50°, 2.81°, and 2.00° respectively. To clearly show the angles to the location of the main peaks, the maximums of the SEDs are normalized to 1. Generally, the angles to the location of the main peaks shift to small values with increasing particle size, which is consistent with the general understanding. However, the angles to the location of the main peaks for $\alpha = 19.0$ and $\alpha = 23.0$ occur in a reversed order. Therefore, the signatures of the SEDs for $\alpha = 19.0$ and $\alpha = 23.0$ are anomalous.