Results in Physics 10 (2018) 22–27

Contents lists available at ScienceDirect

Results in Physics

journal homepage: www.elsevier.com/locate/rinp

# Influence of spheroidal particle shape on particle size characterization by multi-wavelength light extinction method

Zhou Yi, Chen Jun, Yang Hui-nan, Li Tan, Su Ming-xu*

*Institute of Particle and Two-phase Flow Measurement, University of Shanghai for Science and Technology/Shanghai Key Laboratory of Multiphase Flow and Heat Transfer in Power Engineering, University of Shanghai for Science and Technology, Shanghai 200093, China*

ARTICLE INFO

*Keywords:*
Particle size characterization
Multi-wavelength light extinction method
Generalized Lorenz-Mie theory
Extinction spectrum

ABSTRACT

In order to improve the applicability, spheroidal particles are substituted for the spherical particles in the traditional modeling of multi-wavelength light extinction method. The extinction coefficient and extinction spectrum are calculated at different axial ratios under the configuration of the generalized Lorenz-Mie theory. Combining extinction spectrum with regularization inversion algorithm, the influence of particle shape on particle size characterization by multi-wavelength light extinction method is discussed in detail. That is, the arithmetic statistical average and stochastic incidence statistics are employed simultaneously to calculate the extinction spectrum in the visible light range and carry out a validation for submicron particles with a refractive index of 1.33. The corresponding comparison between inversed particle sizes and those of spherical particles yields the resulting inversion deviation within 10% for mono-sized spheroids and 20% for a polydisperse particle system with an axial ratio less than 3, but then the relative deviation may increase significantly with the axial ratio, even up to 50%. It can be seen that for particles of equivalent volume, the spheroidal shape exerts a great influence on particle size characterization, and the assumption of spheroidal particle would become crucial in the cases of axial ratio above 3.

## Introduction

Particulate matter is widely used in the industrial processes, such as coal or liquid fuel combustion, crystallization, and food production, where particle size distribution is directly related to the technical process, product quality, energy consumption, and the safety of production. Therefore, the demand of high accuracy particle size characterization method has become increasingly urged. Accordingly, quite a few methods have been developed in recent years, from ultrasonic spectrometry method, image method to light scattering method. The latter is usually characterized by fast response, high accuracy and non-invasion [1], and subdivided into various techniques. Among them, light extinction method (LEM) has shown its advantages as it is simple to use and its cost is low [2].

In the early study of light extinction method, the monochromatic light has been frequently used for measuring the colloidal concentration. However, it has a very obvious drawback that the measurement results are prone to multi-valued, limiting the size upper range of 1 ~ 2 µm or less. Instead of using monochromatic light, the multi-wavelength extinction method presents a spectra analysis-based technique to determine the particle size distribution and concentration simultaneously. It also demonstrates higher measurement reliability, and wider measurement range, and thus shows great potential in particle size measurement [3]. Moreover, it can be applied in the aerosol size distribution [4], city dust measurement [5], and gas-solid two-phase flow field [6] when it is combined with imaging method. Depending on the wavelength range of light beam, the measurable particle typically ranges from submicron to several microns.

The Lorenz–Mie theory is usually used to explain the phenomenon of light scattering by particles. Thus, the particle size distribution in the laboratory is obtained by analyzing multi-wavelength extinction spectra which contains two implicit conditions: spherical particles are assumed for physical modeling, and transmitted light rather than scattered light information is used for particle characterization. However, in an actual application, the size distribution and the shape of the particle cannot be known in advance, which may bring great difficulties and errors to the inversion of particle size distribution [7]. For example, the ideal spherical particles are very rare no matter in natural environment or in industrial products. Obviously, a large number of irregular particles have brought great difficulties to the mathematical description, which also involves almost all kinds of light scattering methods. Fortunately, the spheroidal particle assumption can be used to

* Corresponding author.
*E-mail address:* sumx@usst.edu.cn (M.-x. Su).

https://doi.org/10.1016/j.rinp.2018.05.003
Received 24 January 2018; Received in revised form 1 May 2018; Accepted 2 May 2018
Available online 09 May 2018

seek a balance between over-simplified shape descriptions and mathematical modeling difficulties. In modeling, it can undoubtedly provide a more rational characterization for the actual particles with various aspect ratios as a flexible shape adjustment parameter, provided that the mathematical modeling and solution can be implemented.

The investigation of light scattering of spheroidal particles has yielded many encouraging achievements. Asano et al. [8] studied the scattering of spheroidal particles on plane waves by separating variable method, proposing a theoretical method to deal with the boundary conditions of the electromagnetic field of spheroidal particles, which was verified to be better in solving the problem of boundary condition. Schulz [9–11] studied the scattering problem of spheroidal particles by using T-matrix method in the field of plane beam incidence. In the subsequent study, Han [12] improved the derivation of boundary conditions and corrected the error parameters in Asano's literatures. Xu et al. [13–22] further investigated the scattering of beams of arbitrary shape, position, and incident angle by the homogeneous spheroid particles. These thorough investigations make the possibility emerge for the calculation of spheroid scattering parameters and even for the further application of extinction spectrum.

On this basis, we propose a modeling method based on the light extinction cross-section of spheroidal particles and explore the influence of shape factors on light extinction spectrum. The contents of this paper are organized as follows: in Section "Principle", the analytical expression of light extinction cross-section and light extinction spectra are derived by using Lambert-Beer's law, as well as the introduction to spheroid coordinate and key scattering parameters calculation. Section "Numerical results of extinction characteristics" is devoted to calculating the effect of the change of the equivalent volume spherical particle axial ratio and discussing the influence of the incident azimuth angle on the light extinction spectrum. In Section "Inversion and results", we obtain the particle size information in the extinction spectra via using the regularization inverse algorithm. The effect of the axis ration, equivalent volume and incident angle on the particle size measurement are consequently studied by comparing inversed sizes with the given nominal ones.

## Principle

### *Light extinction method*

By measuring the extinction spectra of light beam through the discrete particles medium, the particle size distribution is obtained by inversion of the spectral information. The core of the theory is the Lambert-Beer law. Fig. 1 shows that when a collimated incident monochromatic light beam with the strength $I_0$ and wavelength $\lambda$, whose diameter is greatly larger than that of measured particles to meet the conditions of static light scattering, goes through the medium containing numerous spatially stochastically distributed particles, the intensity of the transmitted light due to the scattering and absorption by particles is expressed as follows:

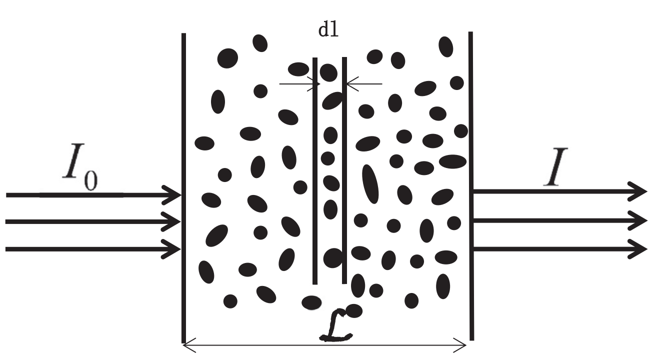


**Fig. 1.** Schematic diagram of the principle of light extinction method.

$$I = I_0 \exp(-\tau L) \tag{1}$$

where, $L$ is the light path, and $\tau$ is the turbidity. If the light scattering of each particle satisfies the non-correlation single scattering, the turbidity of a single scattering particle system in the unit volume is

$$\tau = NC_{ext} = N\frac{\pi}{4}D^2 Q_{ext} \tag{2}$$

where, the extinction cross-section $C_{ext}$ and the extinction coefficient $Q_{ext}$ are the functions of the wavelength $\lambda$ of the incident light, the diameter of the particles $D$ and the refractive index of the particles relative to the surrounding medium $m$. $N$ indicates the particle number in the unit volume. Substituting Eq. (2) into Eq. (1)

$$\ln\left(\frac{I}{I_0}\right) = -NLC_{ext} \tag{3}$$

where, the ratio $I/I_0$ is the transmittance of Light. Obviously, light extinction can be expressed by $1-I/I_0$. The Lorenz–Mie scattering theory, in which the spherical particles are usually assumed, is frequently used to analyze light scattering phenomena and to determine extinction characteristic parameters such as extinction cross-section. However, as shown in Fig. 1, the spherical and non-spherical particles may coexist, the Lorenz–Mie theory and spherical particles assumption would then yield errors, but the degree of influence needs to be investigated and quantified if the light extinction method is expected to be well applied in a real particle system. It should be pointed out that a common simplification operation for spheroids is to used here to define the equivalent size as the diameter of a sphere with the same volume. Then the modeling method based on the extinction cross-section of spheroid particles can be implemented during exploring the influence of shape factors on extinction spectrum. The light extinction characteristic parameters based on the spheroid assumption will be introduced in the next section.

### *Spectral calculation of spheroidal particles*

#### *Spheroidal coordinates*

In order to discuss the shape features of spheroidal particles, the spheroidal coordinates are defined first with the rotation around the oval major axis to form the coordinate system and then the ellipsoidal surface, in which, a point on the spheroid is defined by the angular coordinates $\eta$, the radial coordinates $r$ and the azimuth coordinates $\varphi$. Their ranges are defined as

$$-1 \leqslant \eta \leqslant 1, \quad 1 \leqslant r \leqslant \infty, \quad 0 \leqslant \varphi \leqslant 2\pi \tag{4}$$

Define $f$ as the half-focal length of the spheroid, i.e. the distance between the two focal points of a spheroid.

$$f = a\left[1-\left(\frac{b}{a}\right)^2\right]^{\frac{1}{2}} \tag{5}$$

where, $a$ represents the half-length axis of a rotating spheroid, and $b$ represents the half shaft of the rotating spheroid. Obviously, when $f$ tends to be 0, that is, the focal points of the rotating spheroid coincide, the spheroidal coordinates degenerate into the spherical coordinate system.

#### *Calculation of extinction cross-section, coefficient and spectral*

When plane waves take the polarization angle $\phi = 0°$ and the incident angle $\xi$, the extinction cross-section and extinction coefficient of a single prolate spheroidal particle can be written as follows:

$$C_{ext}(\xi) = -\frac{\lambda}{\pi}\mathrm{Re}\sum_{m,n}[\alpha_{mn}\cdot\sigma_{mn}(\xi) + \beta_{mn}\cdot\chi_{mn}(\xi)] \tag{6}$$

$$Q_{ext}(\xi) = C_{ext}(\xi)/G(\xi) \tag{7}$$