A simple Mie scattering calculation method based on approximate linear model

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Abstract

The light scattering method is the most widely used aerosol measurement method at present, which not only has a wide particle size measurement range, but also has fast measurement speed and good repeatability. In this paper, we analyzed the variation law of the scattered light intensity of a single particle with the incident light wavelength, particle size, surface area and volume, and proposed a function model of the approximate piecewise linear correlation of the scattered light intensity of the aerosol particle and its surface area and volume, simplified the calculation of the particle spectrum distribution from the scattered light intensity, and proposed a method for optimizing the wavelength to detect the scattered light intensity of the aerosol to achieve a fast and accurate inversion of the particle spectrum distribution.

Keywords: Simple Mie scattering calculation, Surface area concentration, Volume concentration

Introduction

With the development and improvement of technology and production process, particle size used in large-scale integrated circuits [1], medical powder spray agents [2] and aerosol transmission route research of infectious viruses [3] has a tendency of decreasing, and the requirements for real-time, convenient and accurate measurement of aerosol particle spectrum are increasing. The light scattering method is the most widely used aerosol measurement method at present, which not only has a wide particle size measurement range, but also has fast measurement speed and good repeatability. Since each particle in the aerosol particle group is small and the distance between particles is more than 3 times of the particle size, it can be regarded as irrelevant scattering, that is, the light scattering intensity of the aerosol particle group can be regarded as the integral/cumulative sum of the scattered light intensity of all particles in the region to be detected.

The scattered light intensity obtained by the detector in one measurement carries the particle size information of all particles. However, it is difficult to completely separate the particle size information in the particle group like the aerodynamic method in the laboratory. Therefore, it is difficult to accurately retrieve the particle spectrum distribution. At the same time, in the classic Mie scattering theory, the relationship between the aerosol particle size and its light scattering intensity needs to be constructed using the Mie scattering coefficient, which involves the calculation of high-order Bessel functions and Hankel functions. The number of cycles calculated by the formula will increase with the increase of the dimensionless particle size, so it is not suitable for accurately solving the particle spectrum distribution in sensor.

Moreover, most of the inversion of the particle spectrum is based on the statistical laws, and the atmospheric aerosol is approximated as Log-normal distribution or Junge distribution, and then the distribution parameters are calculated according to the measurement results. However, there are some deviations between the calculated results based on the preset distribution model and the real distribution of aerosol in real time, resulting in the inaccuracy of the measurement results of particle spectrum distribution.

In this paper, we established a simple Mie scattering model based on the "surface area-volume combined response" of particles, introduced a method to measure the aerosol particle spectrum by scanning the incident light of different wavelengths which similar to the segmentation idea of the aerodynamic method (only suitable for laboratory measurement and damage to particles).

Basic Principles

Mie scattering theory is a strict mathematical solution of Maxwell's equations for uniform spherical particles in a homogeneous medium under the irradiation of monochromatic plane waves. According to Mie scattering theory, the scattered light intensity E_S of a single spherical particle with a distance r to the detector is a function related to the intensity E_0 of the incident light, the dimensionless particle size α (the ratio of particle size x to the incident light wavelength λ), the refractive index m, and the scattering angle θ, that is

$$E_S = \frac{\lambda^2}{8\pi^2 r^2} |S(m,\alpha,\theta)|^2 E_0 \qquad \text{(Eq. 1)}$$

where, $S(m,\alpha,\theta)$ represents the amplitude function of scattered light, and is a non-analytic function composed of a complex high-order Bessel function and Hankel function. According to a large number of statistical results, there is a "three-stage" correspondence between the scattered light intensity of the particle and the dimensionless particle size, that is, when the refractive index of the particles is not considered, when the dimensionless particle size is close to 1 (the incident light wavelength is close to the particle size), the light scattering intensity of the particle is approximately proportional to the volume of the particle; when the dimensionless particle size is greater than 1 (the wavelength is smaller than the particle size), the light scattering intensity of the particle is approximately proportional to the surface area; when the dimensionless particle size is much smaller than 1 (the wavelength is larger than the particle size), the light scattering intensity of the particle is approximately proportional to the particle size to the 6th power, which can be simplified to Rayleigh scattering.

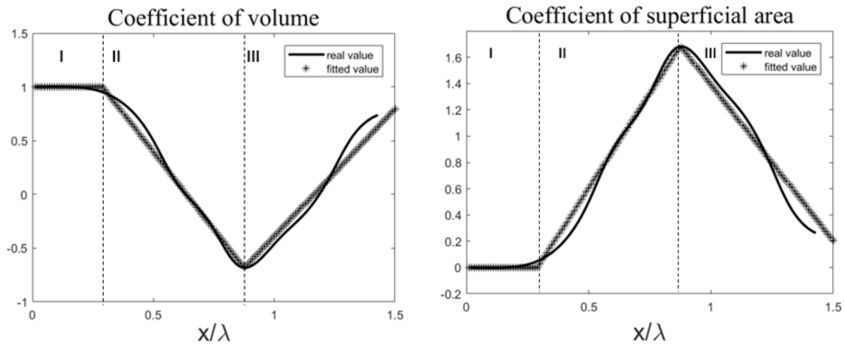
Based on the "three-stage" statistical law, this paper proposes a theoretical model that unifies the three corresponding relations into the same expression, that is, a simple Mie scattering model whose scattered light intensity is only approximately linearly related to its volume and surface area, as shown in Eq. 2:

$$E_S = T_V \times V + T_S \times S \qquad \text{(Eq. 2)}$$

where, V is the particle volume, T_v is the correlation coefficient of particle volume, S is the particle surface area, T_S is the correlation coefficient of particle surface area. The trends of T_v and T_S with the the dimensionless particle are shown in Fig. 1(a) and (b), respectively. For particles of the same particle size, as the wavelength of incident light decreases, the dimensionless particle size of the particles gradually increases, and the volume correlation coefficient T_v first decreases (region II in Fig. 1a) and then increases (region III).

The correlation coefficient T_S increases first (region II in Fig. 1b) and then decreases (region III). The correlation coefficients T_v and T_S both exhibit an approximate piecewise linear trend. In this model, the correlation coefficients T_v and T_S are not directly related to the incident light wavelength or particle size, but only change with the change of the dimensionless particle size.

The scattering response of particles with different particle diameters under different wavelengths of incident light is different. When the wavelength of incident light changes continuously, the intensity of the scattering response of particles to light also changes continuously. In this paper, the idea of replacing the cutting particle size by aerodynamics with the wavelength scanning of incident light is proposed, and the variation law of the scattering response intensity of particles with different particle sizes under continuous wavelength incident light irradiation is analyzed, as shown in Fig. 2.



(a) Volume correlation coefficient changes with dimensionless particle size

(b) Surface area correlation coefficient changes with dimensionless particle size

Fig. 1 In the linear combination relationship between the scattered light intensity of a particle with its surface area and volume, the correlation coefficient varies with the dimensionless particle size.

Among them, the curves of different colors represent the continuously changing wavelength of the incident light, and the wavelength of the incident light corresponding to the curve increases from bottom to top, the range of particle sizes on each curve is the same, the abscissa is the dimensionless particle size, when the incident light wavelength is constant, the change in particle size is equivalent to the change in dimensionless particle size. For incident light of the same wavelength, the change trend of the scattered light intensity of the particles with the dimensionless particle size is to increase first, then approximate to remain unchanged and then decrease, which is consistent with the corresponding relationship of the "three-stage".

At the same time, the larger the incident light wavelength, the stronger the scattered light intensity (the highest curve in Fig. 2 corresponds to the longest incident light wavelength, and the lowest curve corresponds to the shortest incident light wavelength). The scattered light intensity at different wavelengths has a consistent trend with the dimensionless particle size.

Analysis of Fig. 2 shows that for the same dimensionless particle size, the scattered light intensity increases with the increase of the incident light wavelength; at the same time, the longer the incident light wavelength at the same dimensionless particle size, the larger the corresponding particle size, that is, the scattered light intensity of particles with different particle diameters under the action of incident light with continuously changing wavelength will fall into different positions of different curves. Based on this result, the mapping relationship between the wavelength of incident light-particle size-scattered light intensity can be established. Thus, the incident light signals of different wavelengths are used to scan the particles to be measured, and the particle size can be classified according to the change of the scattered light intensity to achieve optical "cutting" of particles.

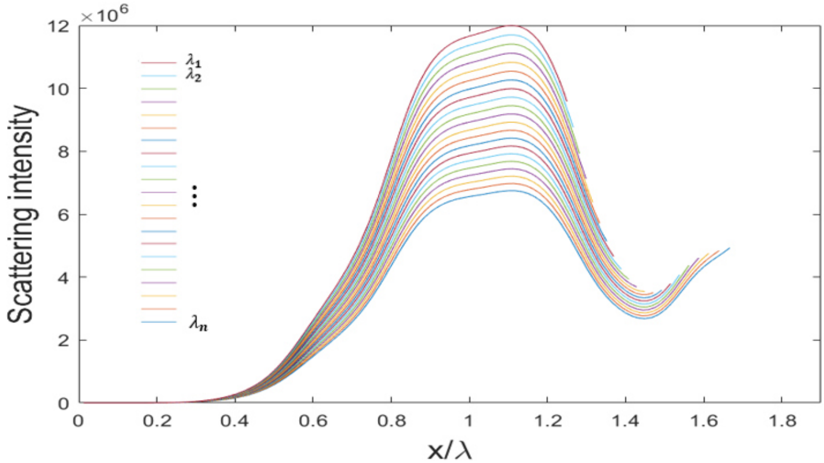


Fig. 2. Scattered light intensities of different particle sizes under irradiation of incident light with continuously varying wavelengths. The curves of different colors represent the continuously changing wavelength of the incident light, and the wavelength of the incident light corresponding to the curve increases from bottom to top. The range of particle sizes on each curve is the same.

On this basis, we established the conversion matrix *T* that depends on the linear combination of surface area and volume between scattered light intensity and particle size. Since the combination coefficient is only related to the dimensionless particle size, for the aerosol particle group, the appropriate incident light wavelength is selected so that the scattered light intensity can be uniquely mapped to each dimensionless particle size. That is, when the curve in Fig. 2 gradually becomes monotonous as λ increases, the row full rank of the conversion matrix *T* can be achieved. In this way, the problem that the classic Mie scattering inversion is difficult to obtain the full rank conversion matrix is solved. Then, the scattered light intensity obtained by the *N* kinds of aerosol particles to be measured under the action of *M* different wavelengths of incident light can be expressed as:

$$E_{M\times 1} = T_{M\times N} W_{N\times 1} \qquad \text{(Eq. 3)}$$

where, $E_{M\times 1} = [e_1, e_2, \cdots, e_M]'$ represents the vector of scattered light intensity under the action of incident light at different wavelengths, $T_{M\times N} = \begin{bmatrix} t_{1,1} & \cdots & t_{1,N} \\ \vdots & \ddots & \vdots \\ t_{M,1} & \cdots & t_{M,N} \end{bmatrix}$ represents the conversion matrix of scattered light intensity that depends only on surface area and volume of particle, $W_{N\times 1} = [w_1, w_2, \cdots, w_N]'$ represents the column vector of the particle size distribution of the aerosol particle group. After the scattered light intensity corresponding to the incident light at each wavelength is measured, the particle size distribution *W* of the particle group can be directly calculated by solving the generalized inverse by the row full rank matrix with sufficient information. The finer grain distribution to be measured, the more types of incident light required. In particular, when *M*=*N*, that is, the wavelength type of incident light is the same as the particle size type to be measured, T_{MxN} is a full-rank square matrix, and the exact distribution of particle spectrum can be obtained by directly multiplying the inverse matrix of T_{MxN} on both sides of Eq. 3.

Simulations and Discussion

The calculation of the classic Mie scattering theory is complicated, and each element in the scattered light intensity conversion matrix T needs to be calculated according to the scattered light intensity of specific particles at a specific wavelength of incident light. For the scattered light intensity conversion matrix T_{MxN} it is necessary to calculate the $M \times N$ times Mie scattering formula to establish a scattered light intensity sensing model of *N* kinds of particles under *M* kinds of incident light, the calculation of this model is very large. Using the simple Mie scattering model based on the “surface area-volume combined response" proposed in this paper, due to the approximate piecewise linearity of the correlation coefficients T_v and T_S, only a minimum of 3 points of light intensity values are needed to obtain a complete $T_{V_{MN}}$, $T_{S_{MN}}$, and then obtain the entire scattered light intensity matrix T_{MxN}, can greatly simplify the calculation complexity, as shown in Eq. 4:

$$t_{ij} = \frac{E_{S_{ij}}}{V_j} = \frac{T_{V_{ij}} \times V_j + T_{S_{ij}} \times S_j}{V_j} = T_{V_{ij}} + \frac{3T_{S_{ij}}}{d_j} \qquad \text{(Eq. 4)}$$

where, *i* represents the i_{th} wavelength, and *j* represents the j_{th} particle size. Based on the classical Mie scattering theory and the simple Mie model proposed in this paper, 100 types of aerosols are scanned with incident light of 7 wavelengths, and the results of inversion of the particle spectrum are shown in Fig. 3. The mean square error of the particle spectrum inversion results based on the classical Mie scattering theory is 0.21 ‰, while the mean square error of the particle spectrum inversion results based on the simple Mie theory is 0.22 ‰. Since the correlation coefficients T_v and T_S are linearly approximated in the simple model, the conversion matrix *T* calculated by Eq. 4 will introduce some errors, but it can be seen from the simulation results that the reconstruction error of this method is only slightly larger than the reconstruction error of classic method, at this cost, the process of calculating and modelling the 700-time Mie scattering formula is simplified to only use the 10-time Mie scattering formula, greatly improving the calculation efficiency.

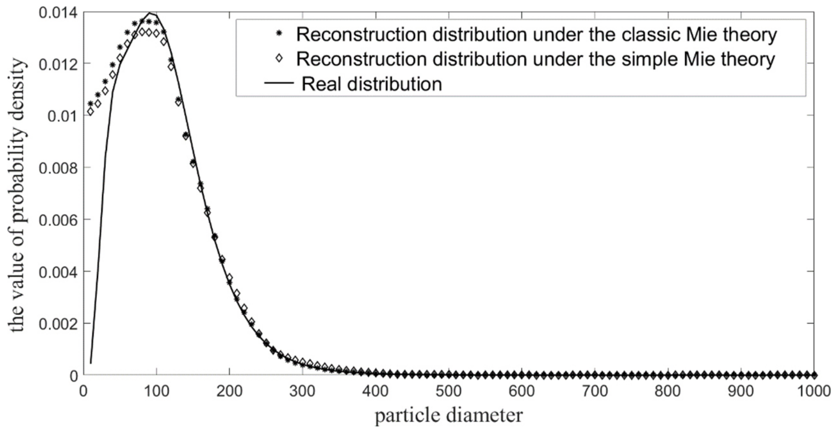


Fig.3. A particle spectrum that satisfies a bimodal log-normal distribution with median values of 70 nm and 130 nm and standard deviations of 1.75 and 1.45, and its reconstruction results under our method.

It can be known from Eq. 3 that when the incident light wavelength type is sufficient, even equal to the number of particle size types to be measured, the conversion matrix T can be made into a full-rank square matrix, and the particle spectrum distribution can be accurately obtained. However, in actual aerosol particle size measurement, only a limited amount of incident light can be used, so it is particularly important to choose the appropriate incident light wavelength.

The optimal wavelength combination of incident light should satisfy the need to carry the particle size information of all particles without redundant information after scattering with the particle group to be measured. It can be seen from Fig. 1 that this condition can be satisfied only by using the wavelength of incident light that can cause the variety of linear changes in the surface area and volume combination coefficient of particles in different segmented regions. According to Fig. 2, with the increase of dimensionless particle size, when the wavelength of incident light is small, it may appear that the scattered light intensity of particles with the same dimensionless particle size under the action of different wavelengths is too close to cannot be distinguished.

Therefore, in the measurement of aerosol particle spectrum, in order to ensure that the scattered light intensity of particles with dimensionless particle size varies significantly under the action of incident light of different wavelengths, the wavelength of incident light adopted should also be appropriately adjusted with the range of particle spectrum to be measured.

Conclusion

In this paper, a method for measuring aerosol particle spectrum with optical "no-damage cutting " based on wavelength scanning of incident light is proposed. By scanning particles with incident light at different wavelengths, the size of the particles is classified by optical "cutting". At the same time, we established a simple Mie scattering calculation model. Under this model, the scattered light intensity of particles can be obtained by the approximate piecewise linear calculation of their volume and surface area, which greatly simplifies the calculation of the scattered light intensity of particles.

On this basis, we used simulation experiments to prove that only a small amount of incident light can be used to achieve fast and accurate particle spectrum reconstruction, then we compared the particle spectrum inversion results of the classical Mie scattering theoretical model and the simple. That is, the reconstruction error of our method is only slightly larger than the reconstruction error of classic method, at this cost, the process is greatly simplified.

Mie scattering model proposed in this paper, which laid a theoretical foundation for the application of the wavelength scanning "cutting" particle size detection method to the portable detector.

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