

RETRIEVAL OF SPHERICAL PARTICLE SIZE DISTRIBUTION WITH AN IMPROVED TIKHONOV ITERATION METHOD

by

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Short paper

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The problem of retrieval for spherical particle size distribution in the independent mode is studied, and an improved Tikhonov iteration method is proposed. In this method, the particle size distribution is retrieved from the light extinction data through the Phillips-Twomey method firstly in the independent mode, and then the obtained inversion results of the particle size distribution is used as the initial distribution and the final retrieved particle size distribution is obtained. Simulation experiments indicate that the spherical particle size distributions obtained with the proposed method coincide fairly well with the given distributions.

Key words: *particle size distribution, light extinction, retrieval, Tikhonov iteration*

Introduction

Atmospheric aerosols play an important role in many atmospheric processes since they have appreciable influence on the Earth's radiation budget, air quality, clouds, and precipitation as well as the chemistry of the troposphere and stratosphere. While the particle size distribution is dependent on the particle coagulation [1], transport [2], nucleation [3], collision [4], atomization [5], breakage [6], and synthesis [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 [8-11]. These techniques mostly contain the light extinction scattering, angle light scattering, diffraction light scattering and dynamic light scattering, and the measurement range of them ranges from nanometer to millimeter. Among these techniques, the light extinction measurement is probably the most attractive one, which can in fact be used for *in situ* monitoring of micron or sub-micron particle systems with a simple optical layout thus providing real time measurement of both particle size distribution and particle concentration.

In light extinction particle sizing, the particle size distribution can be obtained by the light extinction data at multi-wavelengths. The data processing of this technique is actually the solution of Fredholm integral equation of the first kind, which is a classic ill-posed problem. Generally, the inversion methods can be divided into two categories. The first category is

the independent mode algorithm, while the second category is the dependent mode algorithm. However, the dependent mode algorithm is very restrictive because, in many circumstances, the forms of the particle size distributions are unknown, and consequently the independent mode algorithm is preferred, and more and more researchers are interested in studying and adopting this method. The Chahine method and the Phillips-Twomey (PT) method are two commonly used independent mode algorithms [12, 13]. The Chahine method has fast convergence but is noise sensitive. To increase stability, some modification about the Chahine method has been proposed. However, these methods must be performed carefully, and they may lack convergence if the initial distribution is too different from the actual distribution.

The advantage of the PT method is its computational speed and its ability to handle many size classes with stability, but the drawback is evident in that the solutions obtained depend on the accurate determination of the regulation parameters, which vary from case to case. Moreover some constraints, such as the smoothness and positiveness, are to be imposed on the solutions. Motivate by this, we propose an improved Tikhonov iteration method by which the particle size distribution is retrieved from the light extinction data through the PT method firstly in the independent mode, and then the obtained inversion results of the particle size distribution is used as the initial particle size distribution and the final retrieved particle size distribution is obtained by the Tikhonov iteration method.

Theory and computation simulation

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. 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 [14]:

$$\ln \frac{I(\lambda)}{I_0(\lambda)} = -\frac{3}{2} L N_D \int_{D_{\min}}^{D_{\max}} \frac{Q_{\text{ext}}(\lambda, m, D) f(D)}{D} dD \quad (1)$$

where $Q_{\text{ext}}(\lambda, m, D)$ 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 (the ratio of the refractive indices of the particle and the medium) [15, 16], N_D – the total number of particles, the lower and upper integration limits are denoted by D_{\min} and D_{\max} , $f(D)$ – the frequency distribution of a particle system in volume, which is to be determined.

If the spectral extinction is measured at M wavelengths, and the diameter range is divided into N subintervals in $[D_{\min}, D_{\max}]$ interval. The discrete version of eq. (1) is described by $E = Af$ [17] where $E = [\ln(I_1/I_{10}), \dots, \ln(I_M/I_{M0})]$, $A = [A_{ij}]$ is the so-called $M \times N$ weigh matrix, the elements of A is $A_{ij} = -3LN_D Q'_{\text{ext}}(\lambda_i, m, \bar{D}_j)/(2\bar{D}_j)$, $i = 1, \dots, M$, $j = 1, \dots, N$, $f = [f_j]$, $f_j(\bar{D}_j)$ is the volume frequency distribution evaluated in the j -th subinterval $[D_j, D_{j+1}]$, and \bar{D}_j is the midpoint of the j -th subinterval.

For the independent model algorithm, there is no a prior information about the particle size distribution is available and the particle size distribution is retrieved by the discrete liner equation set. It is known that the inversion method according to the spectral extinction is very important, which will influence the precision of the results. One of the most popular numerical inversion methods is the PT method. The solution of $E = Af$ according to the PT regu-

larization is obtained by minimizing: $\min(\|\tau - Kf\|^2 + \gamma \|Lf\|^2)$ where γ is a non-negative regularization parameter, L is a smoothing matrix which is usually a discrete representation of a differential operator. The minimization problem of $\min(\|\tau - Kf\|^2 + \gamma \|Lf\|^2)$ is equivalent to solving the corresponding normal equation $f = (K^T K + \gamma L^T L)^{-1} L^T \tau$. Special care must be taken to choose the regularization parameter γ and the smoothing matrix L . The selection of these two parameters affects the convergence, speed and closeness. In this work, the second derivative operator is applied to the L matrix, and L -curve criterion is used for determining of the regularization parameter γ . However, in some circumstance, the solution in eq. (4) is still unstable and is disturbed easily by the noise. To overcome the oscillations in retrieving the particle size distribution, the Tikhonov iteration method is also considered. The Tikhonov iteration uses the following iterative formula:

$$f_{k+1} = f_k + (K^T K + \gamma H)^{-1} K^T (\tau - Kf_k) \quad (2)$$

where k is the current iteration time.

Table 1 lists the particle size distributions inversion results with different methods. The particle diameter range is set from 0.1 to 10 μm , and in this range it is divided into 100 sub-intervals. The incident wavelengths are used from 0.4 to 0.8 μm with 50 subintervals in the visible light range, and the complex refractive index is 1.33. In tab. 1, the set distributions are assumed to have R-R and L-N distributions, and the initial distribution in the method is obtained by randomly selected way. What we should is to obtain the true particle size distribution by the inversion methods. In tab. 1, we use different inversion methods in order to very the feasibility and variability of the improved Tikhonov iteration method. In order to compare the quality of the retrieved particle size distribution, the following performance index is defined:

$$\eta = \sqrt{\frac{\sum_{j=1}^n (f_j^s - f_j^I)^2}{n}} \quad (6)$$

where f^s is the true distribution and f^I is the retrieved distribution.

Table 1. Particle size distributions inversion results with different methods

Set values	Inversion methods	Inversion errors η
R-R (\bar{D} , k) = (5,8) Noise free	PT	3.25e-05
	Tikhonov iteration	4.03e-05
	Improved Tikhonov iteration	3.89e-05
R-R (\bar{D} , k) = (5,8) $\pm 1\%$ noise	PT	9.52e-02
	Tikhonov iteration	8.17e-01
	Improved Tikhonov iteration	5.39e-02
L-N (u , σ) = (5,1.1) $\pm 1\%$ noise	PT	7.95e-02
	Tikhonov iteration	8.06e-02
	Improved Tikhonov iteration	3.36e-02

According to the inversion results in tab. 1, the improved Tikhonov iteration method gives a slightly smaller relative error and better performance. The results show that the improved Tikhonov iteration method is quite stable and insensitive to the noise levels. Therefore, the improved Tikhonov iteration method can give satisfactory results for the retrieval of spherical particle size distributions in the independent mode.

Conclusions

We propose an improved Tikhonov iteration method to retrieve the spherical particle size distributions in the independent mode. In this method, an estimate solution of spherical particle size distribution is obtained by the PT method, and then the estimate solution of spherical particle size distribution is used as the initial distribution instead of the randomly selected way in the Tikhonov iteration method to retrieve the final spherical particle size distribution. Simulation results indicate that a reasonable representation of the commonly used spherical particle size distributions can be obtained by this inversion approach.

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