Journal of Quantitative Spectroscopy & Radiative Transfer 111 (2010) 2106–2114

Contents lists available at ScienceDirect

Journal of Quantitative Spectroscopy & Radiative Transfer

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

Inverse problem for particle size distributions of atmospheric aerosols using stochastic particle swarm optimization

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A R T I C L E I N F O

Article history:
Received 29 January 2010
Accepted 24 March 2010

Keywords:
Radiative properties
Stochastic particle swarm optimization
Aerosol optical thickness
MIE theory

A B S T R A C T

As a part of resolving optical properties in atmosphere radiative transfer calculations, this paper focuses on obtaining aerosol optical thicknesses (AOTs) in the visible and near infrared wave band through indirect method by gleaning the values of aerosol particle size distribution parameters. Although various inverse techniques have been applied to obtain values for these parameters, we choose a stochastic particle swarm optimization (SPSO) algorithm to perform an inverse calculation. Computational performances of different inverse methods are investigated and the influence of swarm size on the inverse problem of computation particles is examined. Next, computational efficiencies of various particle size distributions and the influences of the measured errors on computational accuracy are compared. Finally, we recover particle size distributions for atmospheric aerosols over Beijing using the measured AOT data (at wavelengths λ=0.400, 0.690, 0.870, and 1.020 μm) obtained from AERONET at different times and then calculate other AOT values for this band based on the inverse results. With calculations agreeing with measured data, the SPSO algorithm shows good practicability.

1. Introduction

Atmospheric aerosols are suspensions of small solid or liquid particles in air. Examples include dust, soot, micro-organisms, spores and plant pollens, and cloud precipitates, hail, sleet, rain and snow, consisting of water and ice, all of which play an important role in the environment because they take part in many physical and chemical processes [1,2]. Atmospheric aerosols can scatter and absorb short-wave solar radiation and long-wave terrestrial radiation, and thus affect the radiation balance of the earth–troposphere system. Thus, atmospheric aerosols are of particular interest in study of atmospheric radiation.

A prominent characteristic of atmospheric aerosol particles is the great temporal–spatial variability of their physical and chemical properties. It is generally believed that the diameters of atmospheric aerosol particles are in the range of a few nanometers (nm) to tens of microns (μm). Concentrations of atmospheric aerosols with diameters smaller than 1 μm range from several tens to several thousand cm^{-3}, while that with diameters larger than 1μm are commonly less than 1 cm^{-3}. An atmospheric aerosol particle can be solid, droplet, or composite particles combining solid and liquid phases. Chemically, they can be either homogeneous or inhomogeneous. Shapes of atmospheric aerosols can vary from the very simple spherical liquid drops to complex non-spherical shapes. In general, life spans in the atmosphere extend from a few days to several weeks. Because residence times of atmospheric aerosol in air are short and their temporal–spatial characteristics vary widely, there has been till date a lack of sufficient data to study the various

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doi:10.1016/j.jqsrt.2010.03.019

influences on global and local climate systems of atmospheric aerosols of different origin and type in the atmosphere.

Countries worldwide have always been developing observational technologies and retrieval methods brought about by combined satellite-based and ground-based optical remote sensing that has in recent years lead to enormous progress in understanding optical characteristics of atmospheric aerosol. One of the key application areas for satellite-based detectors, which include moderate and high resolution imaging spectro-radiometers (MODIS, HIRDLS) [3,4], advanced very high resolution radiometer (AVHRR) [5,6], and multi-angle imaging spectrometers (MISR) [7], is to detect global, including terrestrial, aerosol optical properties. With respect to ground-based remote sensing, one important development is to have established the AERONET sun-photometer global detection network [8]. Aerosol optical properties can then be extracted from data obtained and used to verify satellite-based remote sensing data [9,10]. By these detection means, we can only measure directly optical properties of several bands, but cannot directly obtain the full spectrum data. As the influence of atmospheric aerosols on the terrestrial–atmospheric radiation balance system covers the full spectrum, optical properties of the entire spectrum are therefore necessary to be present. Currently, we can only obtain these properties by indirect methods, that is, from known aerosol particle size distributions and its associated parameters, optical properties of the entire spectrum could be computed. However, obtaining these parameters directly is also very difficult. Therefore, retrieving aerosol particle size distributions $N(r)$ is necessary. Various retrieving techniques have been applied to decrease the degree of ill-condition problem. These include regularization by truncated singular valued decomposition of LIDAR data [11], linear and nonlinear iterative techniques [12,13], damped Gauss–Newton iteration algorithm [14], moment methods [15–17], and computed tomography [18]. Nevertheless, traditional algorithms used for these problems depend on initial values or derivatives which are difficult to resolve accurately by numerical simulations. Random optimal methods such as the genetic algorithm (GA) have been studied to solve reliably global optimal problems [19,20].

The particle swarm optimization (PSO) algorithm, which was introduced by Eberhart and Kennedy [21–23], is able to find global optimum solutions or good approximate solutions, usually without theoretical proof. This is solely due to its ability to explore the search domain with ‘jumps’ from one local solution to others, and thus the global optimum solution can be reached step by step. As reported in Ref. [24], many kinds of problems that can be solved by GA are able to be solved identically by PSO, without suffering the difficulties encountered in GAs. The PSO algorithm has been studied extensively by many researchers in recent years. Ozcan and Mohan [25] have proved that the PSO can guarantee convergence, but not a global optimum. Van den Bergh [26] studied the global convergence (GC) and local convergence of basic PSO and GCPSO, and he pointed out basic PSO could not guarantee global or local convergence.

To guarantee convergence to global optimum solutions, we propose in this paper a modified PSO algorithm with a stochastic selection. To begin with, MIE scattering theory is used to calculate aerosol optical thickness (AOT), which in turn is used as an input for performing the inverse analysis at different wavelengths. A stochastic particle swarm optimization (SPSO) algorithm is adopted to minimize the objective function and estimate parameters that characterize atmospheric aerosol particle size distributions.

2. Methods

2.1. Forward radiation problem

Aerosol particles are assumed for simplicity to be uniform and spherical. For a given aerosol particle size distribution, the calculation of the forward problem is to determine vertical AOTs. The calculation procedure is as follows.

The extinction efficiency factor Q_{ext} and scattering efficiency factor Q_{sca} of spherical particles are given as follows, respectively

$$Q_{ext}(m,\chi) = \frac{C_e}{G} = \frac{2}{\chi^2}\sum_{n=1}^{\infty}(2n+1)\mathrm{Re}\{a_n+b_n\} = \frac{4}{\chi^2}\mathrm{Re}\{S_0\} \quad (1)$$

$$Q_{sca}(m,\chi) = \frac{C_s}{G} = \frac{2}{\chi^2}\sum_{n=1}^{\infty}(2n+1)\left[|a_n|^2+|b_n|^2\right] \quad (2)$$

Here, m is the optical constant of the relevant particles or equivalently the complex refractive index, $m=n-ik$, with n and k denoting the (single) refractive and absorption indices, respectively; χ is the scale parameter, given by $\chi=2\pi r/\lambda$, with r as the particle radius and λ as the wavelength; G is the geometric projected area, $G=\pi r^2$ (m^2 or $\mu\mathrm{m}^2$); the complex numbers a_n and b_n are Mie scattering coefficients, functions of m and χ; C_e and C_s are extinction and scattering cross-sectional areas, respectively. Re denotes the real part of a complex number.

The radiative properties of particle swarm are related to the particle's optical constant, the concentration and the size distribution of particles. The extinction coefficient β, scattering coefficient σ_s, and absorption coefficient κ of particle swarm are defined as

$$\beta = \int_0^{\infty} N(r)C_e\,dr = \pi\int_0^{\infty} r^2N(r)Q_e(r)\,dr \quad (3)$$

$$\sigma_s = \int_0^{\infty} N(r)C_s\,dr = \pi\int_0^{\infty} r^2N(r)Q_s(r)\,dr \quad (4)$$

$$\kappa = \beta - \sigma_s \quad (5)$$

where $N(r)$ is the number density distribution of particles with N_0 of the number density of particles, $N_0 = \int_0^{\infty} N(r)\,dr$.