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Mathematical Modelling for Light Scattering by Spherical Aerosol

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ABSTRACT

Understanding of earth's climates and climate change is governed by radiative processes in the earth-atmosphere system; in which *aerosols* with other particulates play a major role. The radiative properties of atmospheric aerosols are critically dependent on their refractive indices as a function of wavelength and also on their size. Theoretical modelling of light scattering by spherically assumed aerosol particles is always desired not only to gain insight to radiative transfer process but also to supplement ground based experiments. In the present study, we attempt to compute extinction efficiency (Q_e), scattering efficiency (Q_s) and absorption efficiency (Q_a) as function of incident wavelength and size of aerosols. These parameters are then used to compute extinction cross-section (σ_e), scattering cross-section (σ_s) and absorption cross-section (σ_a). A mathematical scheme to deduce above parameters is discussed within the *far-field* (asymptotic) assumption.
Keywords : Aerosols, Lorenz-Mie Theory, Scattering Efficiency, Absorption Coefficient

I. INTRODUCTION

Aerosols are small solid or liquid particles of range of sub-microns to several microns, suspended in the atmosphere. Basically there are two types of Aerosols, *Primary* and *Secondary*. The Primary are directly emitted as particle in the atmosphere and the secondary are originate from chemical reactions [1]. Aerosols play multiple roles in the climate system. They affect the radiation budget directly by scattering and absorption of solar radiation and indirectly, by causing changes in the cloud albedo and lifetime. Due to this the remote sensing of the aerosol properties over land is very difficult task as compared to that over sea or water surface. To make this task more easier, Deuzé et al considered the polarized part of the scattered light in both visible and near infrared spectrum. This has two advantages, (i)Polarized light reflected by land surface is small and independent of wavelength within the considered spectrum. (ii) spatial variability of surface polarized reflection is small then that of the surface reflectance, so the atmosphere is mainly contributing to the Top of the Atmosphere (TOA) polarized signal [2]. This is favourable for remote sensing algorithm and is the motivation behind polarized Remote sensing for retrieval of aerosol.

2. Theoretical Background

2.1 Properties of Atmospheric Aerosols

Many types of particles like aerosols, water droplets, and ice crystals to raindrops, snowflakes, and hailstones are exist in earth's atmosphere. All of these particles are produced by a number of physical and dynamic processes. Atmospheric aerosols reside mainly in the two lowest layers of the atmosphere: the troposphere and the stratosphere [3]. Primary aerosols are directly emitted into atmosphere. Sea spray, mineral dust, volcanic ash, plant and animal debris are the example of primary aerosol. Secondary aerosol are formed in the atmosphere by gas-to-particles conversion processes. SO_2, NO_2 and volatile organic compounds (VOC) are responsible for gas-to-particle conversion, thus producing secondary aerosols [4].

Size is the most fundamental property of an aerosol particle and there is always a distribution of differently sized particles in the atmosphere. When the size of aerosol is less than 2.5μm then it is known as fine mode, if it is greater than 2.5μm then it is known as coarse mode [5]. The fine mode can be further divided into a cluster mode (1–3 nm), a nucleation mode (3–25 nm), an aitken mode (25–100 nm), and an accumulation mode (100–1000 nm) [6].

The earth's radiation budget is the managed by incoming energy from the sun and outgoing energy from the earth. The earth will warm if the Earth and Earth's atmosphere absorb more solar energy than it radiates back to space. The earth will cool if the earth and the earth system radiate more energy to space than it receives from the sun, [7]. When the shortwave emitted from sun is reaches to the earth atmosphere, about one third of the shortwave radiation is reflected back to space by clouds, aerosols, atmospheric molecules and the surface. In addition, a fraction of the incoming solar radiation that is transferred by the atmosphere to the surface is absorbed by greenhouse gases present in the atmosphere. Therefore, only half of the direct shortwave radiation reaches the surface and is absorbed as heat. Due to the ability of greenhouse gases to absorb longwave radiation, the thermal radiation emitted by the surface in turn heats the atmosphere. The thermal radiation emitted by both the atmosphere and the surface is absorbed by clouds and aerosols, so the temperature of atmosphere should be increase [8].

Aerosols have short lifetime and variety of sources, so their effect on climate is much more complex than that of greenhouse gases. Their radiative effects are determined by their concentration, chemical composition, size and shape, are highly variable in both space and time. As a result aerosols affect both regional and global climate [9].

2.2 Interaction of Electromagnetic Radiation with Aerosols

Aerosols influence climate by absorbing and scattering of solar and thermal radiation. These two processes reduce the amount of shortwave radiation reaching the Earth's surface. By reflecting the solar radiation back to space, aerosols contribute to cooling the atmosphere and the surface, whereas absorbing processes lead to positive climate forcing [10].

Scattering and absorption properties of a particle are determined by its chemical composition, size, and the wavelength of the incident radiation. These processes are governed by two wavelength (λ) dependent parameters; the refractive index m and the dimensionless size parameter x:

$$m = m_r - i m_i$$

$$x = \frac{2\pi}{\lambda} a$$

where the real part represents the scattering whereas the imaginary part represents absorption. The real part of the refractive index in the visible spectrum is not very sensitive to the chemical composition. The real refractive index is variable in the range between m_r=1.3-1.65 for most aerosol types and relative humidity while the imaginary part of the index is much more variable, ranging from 1 x 10^{-9} (e.g water droplets) to more than 0.1 in very sooty or iron-rich dust aerosols [11]. In equation 1.2, λ is the wavelength of incident radiation and a is radius of aerosol.

The elastic scattering can be classified further into two: Rayleigh scattering and Mie scattering, depending on the size of the particle as compared to wavelength of the incident radiation. When the particle size is much smaller than the incident wavelength, the scattering is called Rayleigh scattering (x<<1). Blue sky is an excellent example of Rayleigh scattering. When the particle size is same as the incident wavelength, the scattering is called Mie scattering (x˜1). Except in Microwave region, all the particle size is larger than the solar radiation so the Rayleigh scattering theory is not applicable. When the particle size is larger than incident wavelength, the scattering is known as Geometric scattering [5]. Except in Microwave region, all the particle size is larger than the solar radiation so the Rayleigh scattering theory is not applicable [11].

To calculate the efficiency of scattering and extinction efficiency of aerosol we shall assume that shape of aerosol is sphere, the scattered field from the particle is very large and particle is homogeneous there for it is characterized by single refractive index. A good description of Mie theory is provided by Liou K. N and the notation in his book is thus adopted[5]. To compute parameters obtained by using Mie Theory programming language FORTRAN has been used. This code provides accurate results for small and large particles with size parameters.

2.3 Overview of Mie theory

Mie scattering is solution method for light scattering from the sphere, It is applicable for the 0.1<Size parameter(X)<100 (Mie regime). This theory express electric field inside and outside sphere in vector spherical harmonic expansion, which satisfies the Maxwell's equation. Apply boundary condition, match the transverse field at sphere to obtain outgoing spherical wave coefficient which is also known as Mie coefficients a_n, b_n, c_n, d_n. All these coefficients are in general complex quantity. Use series involving a_n, b_n to obtain extinction and scattering efficiency.

Based on the the energy conversation principle, the absorption cross section and the efficiency of the sphere can be evaluated from following equation

$$\sigma_a = \sigma_e - \sigma_s,$$

$$Q_a = Q_e - Q_s \tag{1}$$

Where σ_a is the absorption cross section, σ_e is the extinction cross section, σ_s

Is the scattering cross section, Q_a, Q_e , Q_s is the absorption, extinction and scattering efficiency.

→The scattering cross section is obtained following equation:

$$\sigma_s = Q_s \times \pi \times a^2 \tag{2}$$

where a is the radius of the particle.

→ The extinction cross section is obtained following equation:

$$\sigma_e = Q_e \times \pi \times a^2 \tag{3}$$

→The equation of the scattering efficiency of the sphere with radius r=a should be given below

$$Q_S = \frac{2}{x^2} \times \sum_{n=1}^{\infty} (2n+1)(|a_n|^2 + |b_n|^2) \tag{4}$$

Where x is the size parameter, which is given by

$$x = k \times a = \frac{2\times\pi}{\lambda} \times a \tag{5}$$

Here λ is the wavelength of incident radiation.

The extinction efficiency of the sphere is defined by

$$Q_e = \frac{2}{x^2} \times \sum_{n=1}^{\infty} (2n+1) Re(a_n + b_n) \tag{6}$$

Here a_n, b_n are the Mie coefficients. There are another two Mie coefficients c_n, d_n.

→ Apply boundary condition, match the transverse field at sphere leads to the following expressions of the Mie coefficients [3]

Scattering Mie coefficients

$$a_n = \frac{\psi_n'(y)\psi_n(x) - m\psi_n(y)\psi_n'(x)}{\psi_n'(y)\xi_n(x) - m\psi_n(y)\xi_n'(x)} \qquad b_n = \frac{m\psi_n'(y)\psi_n(x) - \psi_n(y)\psi_n'(x)}{m\psi_n'(y)\xi_n(x) - \psi_n(y)\xi_n'(x)}$$

where, $y = m \times x$

$$\psi_n(x) = \sqrt{\frac{0.5\pi}{x}} \times J_{n+\frac{1}{2}}$$

Here $J_{l+\frac{1}{2}}$ is the spherical Bessel function, which is obtained by following equation

$$\xi_n(x) = \sqrt{\frac{0.5\pi}{x}} \times H^2_{n+\frac{1}{2}}$$

where $H^2_{n+\frac{1}{2}}$ is the Hankel function of second kind

$$H^2_{n+\frac{1}{2}} = \psi_n(x) + i\chi_n(x)$$

where $\chi_n(x)$

$$\chi_n(x) = -\sqrt{\frac{0.5\pi}{x}} N_{n+\frac{1}{2}}(x)$$

where is $N_{n+\frac{1}{2}}(x)$ the Neumann function.

II. RESULTS

To investigate in detail the effect of size of aerosol we select three different wavelength; λ= 450 nm, 460 nm, 800nm. Radius (a) of aerosol is taken equal to 4.30 μm. Through, the solution of a in the present study is arbitrary and represent only a test-case. Further, we have tested and analysed the result for two refractive indices;

(i) Only with real part (m_r).

(ii) Including imaginary refractive index (m_i).

A complete computation is performed in DELL PRECISION 5810 work station on window platform, while FORTRAN-90 code is constructed to program calculations. The FORTRAN code is attached here with as an appendix for reference. To get sound Theoretical insight of the present computational scheme; we first present graphs for various Mie coefficients [Eqs. 7 and 8] appearing in calculation. For example, real and imaginary parts of a_n, b_n are shown separately in figs. 1-4 for refractive index m=1.5+0.05i as a function of size parameter. Mutual comparison between Re(a_n) and Re(b_n) reveal similarity between them except only at intermediate size parameter(~10-25). Being a combination of harmonic function, a_n and b_n show oscillatory behavior.

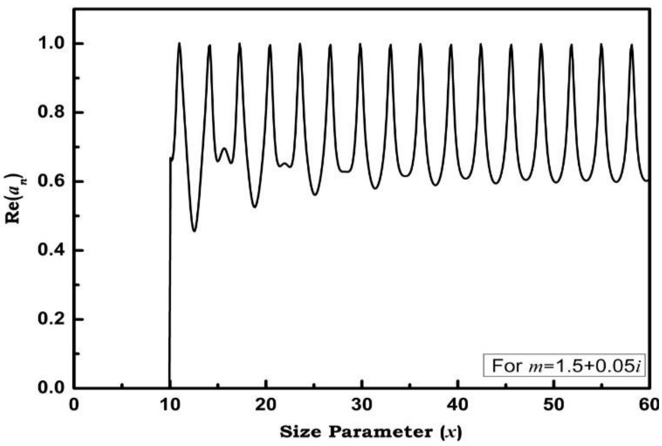

Figure 1. Real part of Mie coefficient (a_n) as a function of size parameter.

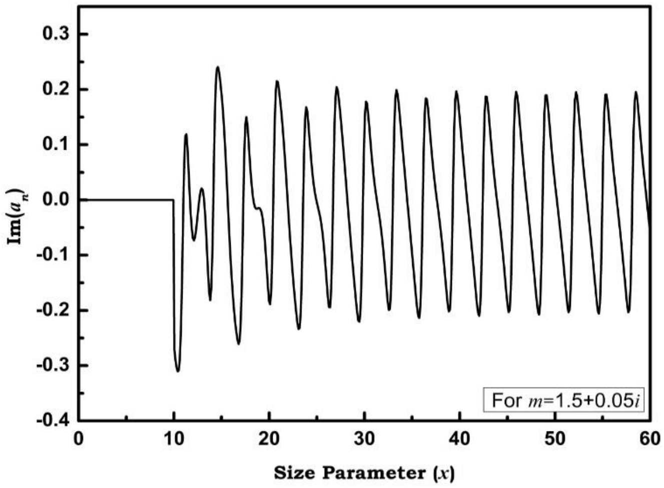

Figure 2. Imaginary part of Mie coefficient (a_n) as a function of size parameter.

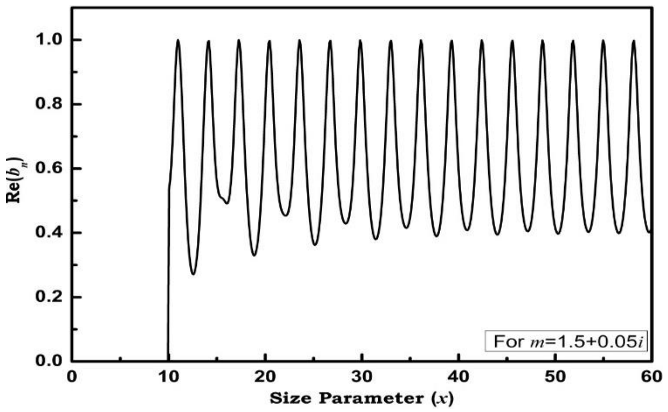

Figure 3. Real part of Mie coefficient (b_n) as a function of size parameter.

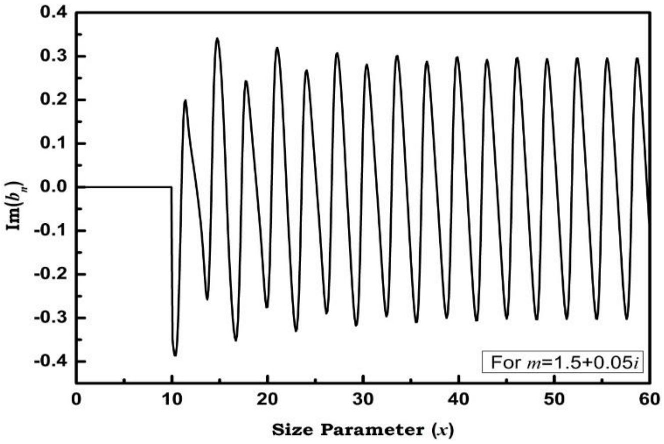

Figure 4. Imaginary part of Mie coefficient (b_n) as a function of size parameter.

Having obtained a_n, b_n as function of size parameter and refractive index; it is possible to calculate

(i) Scattering efficiency (Q_s)

(ii) Extinction efficiency (Q_e)

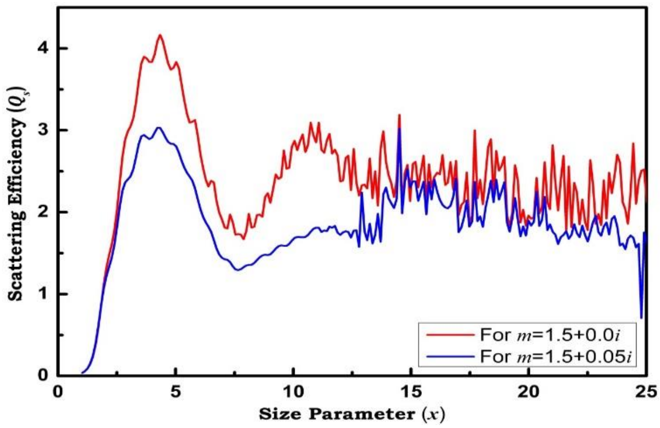

Figure 5 : Scattering efficiency $\boldsymbol{Q_s}$ as a function of size parameter with large n.

In above fig. 4.9 we have also explored the contribution to scattering efficiency (Q_s) from the different poles (i.e up to n=6 in Eq. 3.96) for a selective m=1.5. Fig. 4.9 suggest that in order to have proper convergence in such for multipole expansion to Q_s, one should consider large value of n.

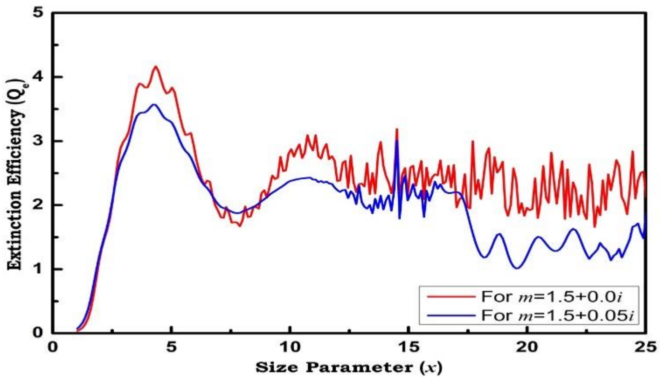

Figure 6: Scattering efficiency $\boldsymbol{Q_e}$ as a function of size parameter with large n.

Figs. 5 and 6 shows the scattering efficiency Q_s and extinction efficiency Q_e as a function of size parameter x for real refractive index 1.5 with imaginary refractive index 0 and 0.05

When the imaginary part is zero, the particle behave as a perfect reflector, there is no absorption. For x<2, Q_s or Q_e is critically dependent on x. The curve reach maximum at relatively small value of x after which they have form damped oscillation. As the particle size increase or the size parameter increase, the damped oscillations settle down to a value of 2 [12].

The position of first maximum and the frequency of oscillation are dependent on the index of refraction m, increasing value of m corresponding to smaller value of x at maximum.

The extinction is due to a combination of blocking of the wave by the particle and interference between incident and scattered waves. Some of the energy beyond the dimensions of the particle is scattered also. According to Babinet's principle, if the particle is very large compared to wavelength, an amount of energy proportional to geometry of cross section is abstracted from beam by scattering and absorption, but a like amount is diffracted out of beamWhen the imaginary part is added in refractive index, true absorption occurs and due to that the dependency of Q_s or Q_e on particle size is modified. As m_i increase from zero, the principle maximum of curve is decreases in magnitude and shift towards the smaller value of x. The amplitude of the secondary oscillations are correspondingly reduced. When the imaginary part is greater than 0.1 the oscillation completely damped out. So as the imaginary part increases the absorption efficiency increases [12].

In the graph of Q_s and Q_e we observe that there are series of maxima, minima and ripples. The ripple structure is caused by scattering resonance of individual partial waves in the multiple expansion of scattered field. The ripple structure become faint as x is large. When the relative indices m is real and it is less than 2, the ripple structure has single periodicity and the position of the peak value of ripple structure is corresponding to those of $\mathrm{Re}(a_n)$ and $\mathrm{Re}(b_n)$. When $m_i < 0.01$ the ripple structure has same approximate period but amplitude of oscillation should be decrease [13].

The major maxima and minima are due to interference. The interference structure has been interpreted as being caused by the interference either of

(i) The forward-scattering light and the incident beam.
(ii) The diffracted and transmitted light wave in near forward direction.

When the imaginary part of m becomes large, $\mathrm{Re}(a_n)$ and $\mathrm{Re}(b_n)$ become small and the interference oscillation amplitudes decrease. The phenomena indicated that the absorption of the sphere becomes strong and the interference become weak when the imaginary part of m become large [14].

III. CONCLUSION

In Q_s and Q_e, when the imaginary part is zero, the aerosol (particle) behaves as a perfect reflector, there is no absorption. The position of first maximum and the frequency of oscillations are dependent on the index of refraction. For a very large particle $Q_s = Q_e$ =2. When the imaginary part is added in refractive index, the principle maximum of curve is decrease in magnitude and shift towards the smaller value of x. During the course of calculation, we have found that when imaginary part is greater than 0.1 (these results are not presented in the dissertation) the oscillation completely damped out. This observation is consistent to given by Chylek.

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