An outline of the method of successive order of scattering (MSOS)

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Abstract

This short note intends to explain an algorithm for multiple light scattering simulations in the hazy atmosphere involving polarized radiation field. It is named MSOS (method of successive order of scattering) and available for severe air pollutions from satellite.

1. Introduction

Increased emissions of anthropogenic atmospheric particles (simply called aerosols hereafter) associated with economic growth can lead to increased concentrations of hazardous air pollutants. Furthermore, yellow dust storms or biomass burnings due to forest fire and/or agriculture burnt field present serious environmental hazards in East Asia, yet their aerosol properties are poorly understood. Aerosol retrieval from the satellite requires radiation simulations in the Earth atmosphere model. Our research group has treated with development of efficient algorithms for aerosol remote sensing including severe hazy episodes (dense concentrations of atmospheric aerosols) [1: Mukai et al. 1992, 2: Mukai et al. 2015]. It is well known that the space observations are particularly available for a systematic monitoring of the Earth with different spatial, spectral, and temporal resolutions. It is of interest to mention that satellite remote sensing is also useful in a case of heavy air pollution episode. While extreme concentrations of aerosols in the atmosphere can prevent aerosol measurements with surface-level photometry, satellites can still be used in such conditions to observe the Earth's atmosphere from space. It is highly likely that large scale air pollution will continue to occur. We know with certainty that much more cross-validation between the space observations and the ground measurements and algorithm improvement are necessary in order to understand aerosols better. In other words, synthetic analysis of aerosols from ground [3: Sano et al. 2003], and computer [4: Takemura et al. 1999, 5: Mukai et al. 2008] as well as space is strongly desired.

Retrieval of optical characteristics of aerosol is achieved by radiation simulation in the Earth atmosphere model. Accordingly various aspects should be taken into account in single and/or multiple light scattering processes concerned with aerosols. This short note intends to explain an algorithm for multiple light scattering simulations in the hazy atmosphere involving polarized radiation field. It has been already achieved aerosol retrieval for haze episodes by using satellite data based on MSOS (method of successive order of scattering). Then this efficient algorithm MSOS is applied here to vector form radiation simulation denoted by Stokes parameters (I, Q, U, V) or (Il, Ir, U, V) in the optically thick atmosphere. In other words, this work proposes an algorithm for radiation simulation in the Earth atmosphere consisting in the polarized radiation field. Because the satellite polarimetric sensor POLDER has shown that the spectro-photopolarimetry is very useful for the observation of aerosols [6: Deschamps et al. 1994]. JAXA has been developing the new Earth observing satellite GCOM-C, which will board the polarimetric sensor SGLI (second-generation global imager) in 2017. The

SGLI has two polarization channels at near-infrared wavelengths of 670 and 870 nm. The aerosol models have been developed using the accumulated measurements during more than ten years provided with the world wide aerosol monitoring network (AERONET) [7: Dubovik et al. 2002, 8: Omar et al. 2005].

The remainder of this article is organized as follows: Section 2 is the brief interpretation of the radiation simulations for remote sensing. Section 3 is the main body of this work on explanation of the method of successive order of scattering (MSOS) for a semi-infinite atmosphere.

2. Radiation simulations for remote sensing

Algorithms for aerosol retrieval with remote sensing data are divided into three parts in brief as: 1) satellite data analysis, 2) aerosol modelling, and 3) multiple light scattering calculations in the Earth atmosphere model which are called radiative transfer simulations. The radiative transfer simulations incorporate the Rayleigh scattering by molecules and Mie scattering by aerosols in the atmosphere, and reflection by the Earth surface into account. Thus the aerosol properties are estimated by comparing satellite measurements with the numerical values of radiation simulations in the coupled atmosphere-surface model. It is noted that the precise simulation of multiple light-scattering processes is necessary, and needs a long computational time especially in the polarized radiation field. Therefore, efficient algorithms for radiative transfer problems are indispensable to retrieve aerosols from space.

The space-borne sensors measure upwelling radiance at the top of the atmosphere (TOA), and it is known that incident solar light interacts multiply with atmospheric particles. Now function $\mathbf{I}$ (τ, Ω) is defined to be the specific intensity vector at the optical depth τ in the direction of Ω, given by $\Omega = (\mu, \varphi)$ and $d\Omega = d\mu\, d\varphi$, where μ is the cosine of the zenith angle θ (i.e. $\mu = \cos\theta$) and φ is the azimuth angle. That is to say $\mathbf{I}$ (τ, Ω) is the function of τ, the optical depth, of μ, the cosine of angle, θ, between the outward normal of the plane parallel medium and the direction of the light, and of the azimuth angle, φ, of the light measured from a fixed direction. Also, $\tilde{P}(\Omega, \Omega')$ is the matrix of μ, μ', φ, and φ', similarly defined quantities on incident and scattered ray. Hereafter we shall use an abbreviation that Ω stand for (μ, φ). The standard problem in the functions for a given medium with constant or vertically-resolved single scattering albedo ω. The basic physical concept is simple. The intensity $\mathbf{I}$ (τ, Ω) is reduced by $e^{-d\tau}$ after traversing over an optical thickness $d\tau$ at a wavelength λ. The equation of radiative transfer describes this circumstance as [9: Chandrasekhar 1960]

$$\mu \frac{d\,\mathbf{I}(\tau, \Omega)}{d\,\tau} = \mathbf{I}(\tau, \Omega) - \frac{\omega}{4\pi}\int \tilde{P}(\Omega, \Omega') \cdot \mathbf{I}(\tau, \Omega')\,d\,\Omega', \tag{1}$$

where ω and $\tilde{P}$ represent albedo and phase matrix for single scattering, respectively. The integration is carried out over all solid angle. The vector $\mathbf{I}$ is defined to be the four dimensional representing the polarized radiation field,

$$\mathbf{I} = (I_l, I_r, U, V) \text{ or } (I, Q, U, V) \tag{2}$$

These four quantities represent the Stokes parameters, and the 4 × 4 matrix $\tilde{P}$ represents the phase relation in the light scattering. The boundary conditions for the standard problem are (i) at the top of the medium, $\tau = 0$, there is no radiation falling except in direction $-\mu_0$. (ii) at the bottom of the medium, $\tau = \tau_0$, for the finite medium, no radiation incident on the medium at all (namely free surface), or for the semi-infinite case.

Eq. (1) with the boundary conditions above can be rewritten in terms of source function $\mathbf{J}$ (τ, Ω),

$$\mathbf{J}(\tau, \Omega) = \frac{\omega}{4\pi}\int \tilde{P}(\Omega, \Omega') \cdot \mathbf{I}(\tau, \Omega')\,d\,\Omega', \tag{3}$$

as

$$\mathbf{J}(\tau, \Omega) = \omega\Lambda_\tau\{\mathbf{J}(\tau, \Omega)\} + e^{-\tau/\mu_0}, \tag{4}$$

where Λ denotes the usual Λ-operator for semi-infinite or finite medium [10: Busbridge 1960]. The physical meaning of this equation is clear. The first and second terms in Eq. (4) corresponds to the probability of multiple scattering and direct transmission over the distance τ in direction μ_0, respectively [11: Sobolev 1963]. The reflection and transmission functions are obtained through Laplace transform of **J** (τ, Ω).

A more direct approach to the problem is to formulate a set of functional equations for the reflection and transmission functions. The principle of invariance stated originally by Ambartsumian and examined extensively by Chandrasekhar is elegant to attack the problem. The integral equation for the reflection function in case of semi-infinite medium which is related to H-function is given by Chandrasekhar. And, in case of finite medium, the reflection and transmission functions are related to X and Y function and the equations for them are given also by Chandrasekhar.

3. The method of successive order of scattering

3-1 The successive scattering approximation

The idea of successive order of scattering is fundamentally related to the probabilistic approach to the theory of radiative transfer. Many papers have been written in this field and much progress has been made. However, since it is too heavy to review all of these here, only a narrow field which concerns directly to the method of successive order of scattering (MSOS) is simply reviewed in this section.

Eq. (4) suggests an iterative solution of a form in n times scattering case [11: Sobolev 1963],

$$\mathbf{J}_n(\tau,\ \Omega) = \omega\Lambda_\tau\{\mathbf{J}_{n-1}(\tau,\ \Omega)\} + e^{-\tau/\mu_0} \quad n \geq 1, \tag{5}$$

$$\mathbf{J}_0(\tau,\ \Omega) = e^{-\tau/\mu_0}, \tag{6}$$

and

$$\mathbf{J}(\tau,\ \Omega) = \sum_{n=0}^{\infty} \omega^n \mathbf{J}_n(\tau,\ \Omega), \tag{7}$$

which represents the expansion of **J** (τ, Ω) in terms of ω^n, namely Neumann series solution. The physical meaning of these equations is obvious. Eq. (5) gives the source function which is composed of photons scattered once or more, and Eq. (6) for photons not experienced scattering. The entire source function given by Eq. (7) is a weighted sum of these source functions by ω^n, since a photon survives with probability ω at a single act of scattering.

It is easy to treat Eq. (7) with only first two or three terms [12: van de Hulst 1949]. However, the numerical computation must be consulted beyond the 3rd order. The direct treatment on the reflection and transmission functions in this respect is also possible. We can derive a set of recurrence relation between the n-th order function add the lower ones from some mathematical manipulation starting from Eq. (6) or from some physical reasoning. The problem in this successive approximation method is the slowness of the convergence in Eq. (5). When ω is small compared to one, or when the thickness of the medium is small, the computation is easy. However, when $\omega \rightarrow 1$ and medium becomes semi-infinite, the labour is formidable. This problem will be considered later.

3-2 Brief concept of MSOS

It seems not trivial to examine if the successive scattering technique mentioned in the previous section is useful to the radiation field reflected from the optically semi-infinite atmosphere model [13: van de Hulst 1963, 14: Sovolev 1968, 15, 16: Uesugi&Irvine 1969, 1970]. This technique is available for the aerosol episodes. Then we treat with the radiation simulation algorithms in a semi-infinite polarized radiation field. Suppose there is an incident radiation of flux **F** in direction (μ_0, φ_0) falling on the top of a semi-infinite atmosphere, and the flux is supposed to be polarized as

$$\mathbf{F} = (F_l,\ F_r,\ F_U,\ F_V) \tag{8}$$

Let the diffusely reflected radiation intensity vector be **I** (Ω). Decomposing **I** (Ω) into the successively scattered intensity $\mathbf{I}$ (n: Ω) from the same reasoning of Eq.(7), i.e.,

$$\mathbf{I}(\Omega) = \sum_{n=1}^{\infty} \omega^n \mathbf{I}(n : \Omega). \tag{9}$$

In other words, the above diffusely reflected intensity denotes the emergent intensity from TOA (τ = 0) and it is derived by using reflection matrix $\tilde{R}$

$$\mathbf{I}(\Omega) = \frac{1}{4\pi}\int_{-} \tilde{R}(\Omega, \Omega') \cdot \mathbf{F}(\Omega')\mu' \, d\Omega', \tag{10}$$

where the integration covers inward hemisphere and the reflection matrix is expressed by the Stokes parameters

$$\tilde{R} = \begin{pmatrix} R_{ll} & R_{lr} & R_{lU} & R_{lV} \\ R_{rl} & R_{rr} & R_{rU} & R_{rV} \\ R_{Ul} & R_{Ur} & R_{UU} & R_{UV} \\ R_{Vl} & R_{Vr} & R_{VU} & R_{VV} \end{pmatrix} \tag{11}$$

Also we can define the n-th order reflection in eq.(11) as:

$$\tilde{R}(\Omega, \Omega_0) = \sum_{n=1}^{\infty} \omega^n \tilde{R}(n : \Omega, \Omega_0), \tag{12}$$

where n is the number of scattering. The matrix $\tilde{R}$ (n: Ω, Ω_0) is the n-th order reflection describing the radiation emerging at the TOA after scattering n times within the atmosphere. That is to say reflection $\tilde{R}(\Omega, \Omega_0)$ can be calculated as the Neumann series of the nth-order of reflectance $\tilde{R}$ (n: Ω, Ω_0).

The equation for the n-th order of reflection will be derived here as follows. We have a defining equation for $\tilde{R}$ (1: Ω, Ω_0) as

$$\mathbf{I}(1 : \Omega) = \frac{1}{4\pi\mu}\int_{-} \tilde{P}(\Omega, \Omega') \cdot \mathbf{F}(\Omega') d\Omega' \tag{13}$$

where the integration is over inward half space. Now, when a thin layer of thickness Δ is added at the TOA of this semi-infinite medium, the radiation field becomes

$$\mathbf{I}(1 : \Omega, \Delta) = \frac{1}{4\pi}\int_{-} \tilde{R}(1 : \Omega, \Omega') \cdot \mathbf{F}(\Omega')\mu' \, d\Omega' + \frac{1}{4\pi}\int_{-}\left(1 - \frac{\Delta}{\mu}\right)\tilde{R}(1 : \Omega, \Omega') \cdot \left(1 - \frac{\Delta}{\mu'}\right) \mathbf{F}(\Omega')\mu' \, d\Omega' \tag{14}$$

or

$$= \frac{\Delta}{4\pi\mu}\int_{-} \tilde{P}(\Omega, \Omega') \cdot \mathbf{F}(\Omega') d\Omega' - \frac{\Delta}{4\pi}\int_{-}\left(\frac{1}{\mu} - \frac{\Delta}{\mu'}\right)\tilde{R}(1 : \Omega, \Omega') \cdot \mathbf{F}(\Omega')\mu' \, d\Omega' + \frac{1}{4\pi}\int_{-} \tilde{R}(1 : \Omega, \Omega') \cdot \mathbf{F}(\Omega')\mu' \, d\Omega'. \tag{15}$$

Since the thickness (Δ) of added layer is very thin, the intensity $\mathbf{I}$ (1: Ω) in Eq. (13) must be equal to $\mathbf{I}$ (1: Ω, Δ) given by Eq.(15). As a result, we get the following relation

$$\int_{-}\left(\frac{1}{\mu} - \frac{\Delta}{\mu'}\right)\tilde{R}(1 : \Omega, \Omega') \cdot \mathbf{F}(\Omega')\mu' \, d\Omega' \cong \frac{1}{\mu}\int_{-} \tilde{P}(\Omega, \Omega') \cdot \mathbf{F}(\Omega') d\Omega'. \tag{16}$$

Now, letting

$$\mathbf{F}(\Omega') = \delta(\mu - \mu_0) \cdot \delta(\varphi' - \varphi_0)\mathbf{E}, \tag{17}$$

where $\mathbf{E}$ is the unity vector (1, 1, 1, 1), we obtain from eq. (16)

$$(\mu + \mu_0)\tilde{R}(1 : \Omega, \Omega_0) = \tilde{P}(\Omega, \Omega_0). \tag{18}$$

In a similar manner as above, we have the second order one as

$$\mathbf{I}(2 : \Omega) = \frac{1}{4\pi}\int_{-} \tilde{R}(2 : \Omega, \Omega') \cdot \mathbf{F}(\Omega')\mu' \, d\Omega' \tag{19}$$

Under the same reasoning as above, we get

$$\begin{aligned} &\mathbf{I}(2 : \Omega, \Delta) \\ &= \int_{-}\frac{d\Omega''}{4\pi}\int_{-}\frac{d\Omega'}{4\pi}\left(1 - \frac{\Delta}{\mu}\right) \\ &\tilde{R}(1 : \Omega, \Omega') \cdot \Delta\tilde{P}(\Omega', \Omega'') \cdot \mathbf{F}(\Omega'') \\ &+ \int_{-}\frac{d\Omega''}{4\pi}\int_{-}\frac{d\Omega'}{4\pi}\frac{\Delta}{\mu}\tilde{P}(\Omega, \Omega') \cdot \\ &\tilde{R}(1 : \Omega', \Omega'') \cdot \left(1 - \frac{\Delta}{\mu''}\right)\mathbf{F}(\Omega'')\mu'' \\ &+ \int_{-}\frac{d\Omega''}{4\pi}\left(1 - \frac{\Delta}{\mu}\right)\tilde{R}(2 : \Omega, \Omega'') \cdot \left(1 - \frac{\Delta}{\mu''}\right)\mathbf{F}(\Omega'')\mu'' \\ &= \Delta\int_{-}\frac{d\Omega''}{4\pi}\int_{+}\frac{d\Omega'}{4\pi}\tilde{R}(1 : \Omega, \Omega')\tilde{P}(\Omega', \Omega'') \cdot \mathbf{F}(\Omega'') \\ &+ \Delta\int_{-}\frac{d\Omega''}{4\pi}\int_{+}\frac{d\Omega'}{4\pi}\tilde{P}(\Omega, \Omega') \cdot \\ &\tilde{R}(1 : \Omega', \Omega'') \cdot \mathbf{F}(\Omega'')\mu'' \\ &- \Delta\int_{-}\frac{d\Omega''}{4\pi}\left(\frac{\Delta}{\mu} + \frac{\Delta}{\mu''}\right)\tilde{R}(2 : \Omega, \Omega'') \cdot \mathbf{F}(\Omega'')\mu'' \\ &+ \frac{1}{4\pi}\int_{-}\tilde{R}(2 : \Omega, \Omega') \cdot \mathbf{F}(\Omega')\mu' \, d\Omega'. \end{aligned} \tag{20}$$

From Eqs. (19) and (20), and by applying Eq. (17), we have

$$(\mu + \mu_0)\tilde{R}(2 : \Omega, \Omega_0)$$

$$= \frac{\mu}{4\pi}\int_{+} \tilde{R}(1:\Omega,\Omega')\cdot\tilde{P}(\Omega',\Omega_0)d\Omega' + \frac{\mu_0}{4\pi}\int_{+}\tilde{P}(\Omega',\Omega_0)\cdot\tilde{R}(1:\Omega,\Omega')d\Omega'. \quad (21)$$

Generally, the equation for the n-th order $\tilde{R}(n)$ ($n\geq 3$) can be derived in a similar manner as shown above. The n-th order emergent intensity I (n, Ω) is defined as

$$\mathbf{I}(n:\Omega) = \frac{1}{4\pi}\int_{-}\tilde{R}(n:\Omega,\Omega')\cdot\mathbf{F}(\Omega')\mu' \, d\Omega' \quad (22)$$

Then

$$\mathbf{I}(n:\Omega,\Delta)$$
$$= \int_{-}\frac{d\Omega'}{4\pi}\int_{-}\frac{d\Omega''}{4\pi}\left(1-\frac{\Delta}{\mu}\right)$$
$$\tilde{R}(n-1:\Omega,\Omega')\Delta\tilde{P}(\Omega',\Omega'')\cdot\mathbf{F}(\Omega'')$$
$$\int_{+}\frac{d\Omega'}{4\pi}\int_{-}\frac{d\Omega''}{4\pi}\frac{\Delta}{\mu}\tilde{P}(\Omega,\Omega')\cdot$$
$$\tilde{R}(n-1:\Omega',\Omega'')\cdot\left(1-\frac{\Delta}{\mu''}\right)\mathbf{F}(\Omega'')\mu''$$
$$+\sum_{n'=1}^{n-2}\int_{-}\frac{d\Omega'}{4\pi}\int_{+}\frac{d\Omega''}{4\pi}\int_{-}\frac{d\Omega'''}{4\pi}\left(1-\frac{\Delta}{\mu}\right)\cdot$$
$$\tilde{R}(n':\Omega,\Omega')$$
$$\times\Delta\tilde{P}(\Omega',\Omega'')\cdot$$
$$\Delta\tilde{R}(n-n'-1:\Omega'',\Omega''')\left(1-\frac{\Delta}{\mu'''}\right)\mathbf{F}(\Omega''')\mu'''$$
$$+\int_{-}\frac{d\Omega''}{4\pi}\left(1-\frac{\Delta}{\mu}\right)\tilde{R}(n:\Omega,\Omega''')\cdot\mathbf{F}(\Omega''')\mu'''. \quad (23)$$

Thus we have

$$(\mu+\mu_0)\tilde{R}(n:\Omega,\Omega_0)$$
$$= \frac{\mu}{4\pi}\int_{-}\tilde{R}(n-1:\Omega,\Omega')\cdot\tilde{P}(\Omega',\Omega_0)d\Omega'$$
$$+\frac{\mu_0}{4\pi}\int_{+}\tilde{P}(\Omega,\Omega')\cdot\tilde{R}(n-1:\Omega',\Omega_0)d\Omega'$$
$$= \frac{\mu}{4\pi}\frac{\mu_0}{4\pi}\sum_{n'=1}^{n-2}\int_{-}\int_{+}\tilde{R}(n':\Omega,\Omega')\cdot\tilde{P}(\Omega',\Omega'')$$
$$\times\tilde{R}(n-n'-1:\Omega'',\Omega_0)d\Omega'\,d\Omega''. \quad (24)$$

Thus the polarized radiation field reflected from the optically semi-infinite atmosphere is calculated based on Eq. (12) by utilizing Eqs. (18), (21) and (24). The space-borne sensors measure upwelling radiance at the top of the atmosphere (TOA), namely the reflectance ($\tilde{R}$)) from the Earth' s atmosphere. We name this technique MSOS (method of successive order of scattering) as a successive scattering method for semi-infinite atmosphere.

The single scattering matrix $\tilde{P}(\Omega,\Omega_0)$ can be expanded in a Fourier series with respect to the azimuth angle as

$$\tilde{P}(\Omega,\Omega_0)\equiv\tilde{P}(\mu,\varphi,\mu_0,\varphi_0)$$
$$=\tilde{P}^{0}(\mu,\mu_0)+2\sum_{l=1}^{\infty}$$
$$[\tilde{P}_c^{(l)}(\mu,\mu_0)\cos l(\varphi-\varphi_0)$$
$$+\tilde{P}_s^{(l)}(\mu,\mu_0)\sin l(\varphi-\varphi_0)] \quad (25)$$

Similarly the reflection matrix ($\tilde{R}$) can be also expanded in a Fourier series

$$\tilde{R}(n:\Omega,\Omega_0)\equiv\tilde{R}(n:\mu,\varphi,\mu_0,\varphi_0)$$
$$=\tilde{R}^{0}(n:\mu,\mu_0)+2\sum_{l=1}^{\infty}$$
$$[\tilde{R}_c^{(l)}(n:\mu,\mu_0)\cos l(\varphi-\varphi_0)$$
$$+\tilde{R}_s^{(l)}(n:\mu,\mu_0)\sin l(\varphi-\varphi_0)] \quad (26)$$

The equations for Fourier coefficients corresponding to equations (18), (21) and (24) are derived. It is clear that computation time is saved by using the Fourier expansion. However Eq.(12) shows the problem of slowness convergence of MSOS in ω→1. After several improvements have been made on the present form, the MSOS is available for data analysis of the satellite data in a global scale.

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