

Theoretical Studies of Time Dependent/Independent Radiative Transfer Including Inelastic Scattering for both Active and Passive Sources

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LONG-TERM GOALS

We wish to develop the theoretical and computational groundwork for a new and innovative program for the remote detection and characterization of both organic and inorganic aerosols using both active (lidar) and passive techniques. This aerosol study should be very beneficial to the Navy in the areas of communications, high power laser transmission, air-sea interactions, and standoff biological detection methods. We also want to continue our collaborative program in polarimetry with the group in Minsk headed by Dr. Eleonora Zege.

OBJECTIVES

We will incorporate the full Mueller matrix formulation in this study to extract *everything* optically that can be extracted from the scattering and fluorescing aerosols. This study will also include the use of state-of-the-art techniques to calculate the single scattered Mueller matrix (SSMM) for both single particles as well as ensembles of particles that have different morphology and optical properties. We will show how to extend the SSMM into an "effective" multiple scattering Mueller matrix (MSMM) when multiple scattering has to be taken into account. We will also show that by using the MSMM it may be possible to not only determine particle optical properties and number densities but particle morphology as well. We will then determine which Mueller matrix elements or combination of them are most effective for unique aerosol signatures. We are also continuing to explore new and exciting methods for standoff detection of harmful biological aerosols such as anthrax spores.

APPROACH

The success of this study for an active system depends on having programs to accurately calculate the complete time-resolved Mueller matrix for a realistic source-receiver geometry for a medium consisting of atmospheric gasses, clouds, and aerosols. We have already developed very powerful Monte Carlo programs that will calculate the multiple scattering Mueller matrix for any inhomogeneous atmosphere-ocean system which may contain a stochastic surface such as a dielectric interface separating the atmosphere from either a body of water or solid surface. These programs must be capable of handling not only backscattering (monostatic configuration), which is the most common mode of operation of lidar systems, but must also be able to handle any bistatic situation where source and receiver are at positions which will optimize the distinguishing feature of the aerosol under study.

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We have modified our existing state-of-the-art Monte Carlo codes to be able to handle both time dependent and time independent active sensing. For the lidar codes we now have the flexibility to have any source-receiver geometry with arbitrary field of view (FOV) for the detector. We have also extended our Monte Carlo method to full Mueller matrix calculations for a spherical shell atmosphere. This is very important when one cannot use the plane parallel approximation and earth curvature effects become important which is a problem when tracking ICBM's over the horizon.

In order to run our Monte Carlo program, we still need the SSMM for the aerosols and other constituents comprising the atmospheric system. The actual experimental Mueller matrix data for aerosols of different shapes and optical properties are quite sparse at best, therefore we have to develop our own computer codes to give us this data. Many aerosols whether from soils, minerals or organics can be highly nonspherical with large aspect ratios. Trying to model them with any type of equivalent sphere approximation can lead to substantial errors as has been pointed out by Mischenko et al.^{1,2} We have recently published a much more thorough investigation showing that regardless of the type of spherical approximation used, substantial errors can be incurred for many different particle shapes³. There have been many techniques introduced to solve the problem of electromagnetic scattering from irregular particles (for an excellent summary of the methods the reader should see Mischenko, et al.⁴) the most notable of which are the discrete dipole approximation (DDA), the T-matrix approach, and the finite difference time domain method (FDTD). We have a good deal of experience with the DDA; however, even though it is capable of modeling any shape, it is quite limited to size parameters usually less than ten and also suffers from lack of accuracy in the Mueller matrix elements involving phase information. The T-matrix approach is very powerful and is able to achieve size parameters in excess of one hundred; however, it is not well suited for particles with sharp corners and edges where an inordinately large number of vector spherical wave functions may be needed. The FDTD method has a long and rich history beginning with the work of Yee⁵. This method is applicable to any particle shape and inhomogeneity as well as handling any type of incident beam. The application of this method to effectively calculate light scattering properties from dielectric aerosols at a single frequency with a variety of shapes has been carried out by Yang and Liou⁶; however, virtually all comparisons were done on phase functions, the (1,1) element of the Mueller matrix, and is the least sensitive to numerical errors compared to all the other Mueller matrix elements. We have developed a new method using fourth order symplectic schemes to solve this problem and preliminary results are very encouraging. We want to extend the FDTD method to handle both dispersive and tensor permittivities as well. The reason being is that if one is using short pulsed sources the frequency spectrum can be quite wide and in most instances the permittivity will be a function of frequency and this behavior must be accounted for. Also most organic molecules and substances are optically active and therefore the permittivity will no longer be a scalar but will become a tensor. Both of these additions will involve extensive modification of the FDTD method as it presently exists.

These projects are being worked on by Yu You, Julie Slanker, and Lei Bi. Yu You and Lei Bi are both working toward their Ph.D's in physics and Julie Slanker will receive her M.S. degree in December.

WORK COMPLETED

a) We have completed a study of the single scattering properties of the family of Platonic solids, i.e. tetrahedron, cube, octahedron, dodecahedron and icosahedron, using a geometrical-optics ray-tracing technique). A paper on this study has appeared in JQSRT, 106, 595-603, (2007).

- b) We have developed a fast infrared radiative transfer model (RT) using as a basis the adding–doubling principle, hereafter referred to as FIRTm-AD, to facilitate the forward RT simulations involved in hyperspectral remote-sensing applications under cloudy-sky conditions. A paper on this study has appeared in JQSRT, 105 243–263, (2007)
- c) We have completed a study where we compared the finite-difference time domain (FDTD) solutions with the corresponding T-matrix results for light scattering by circular cylinders with specific orientations. The FDTD method was then utilized to study the scattering properties of horizontally oriented hexagonal ice plates at two wavelengths, 0.55 and 12 μm . A paper on this work has appeared in JQSRT, 100, 91-102, (2006)
- d) We have completed the design for a flow-through integrating cavity absorption meter. This instrument, in principle, is capable of measuring the spectral optical absorption coefficient of natural waters in situ independently of scattering effects. A paper on this work has appeared in Applied Optics, 45, 8990-8998, (2006).
- e) We have completed a study of the use of short illuminating pulses in a cavity with highly reflecting walls and studying the temporal decay of the radiation in the cavity as a means to measure weak absorption in the cavity. A paper on this work has appeared in Applied Optics, 45, 9053-9065, (2006)
- f) We have completed a study of a numerical approach for the calculation of the internal dipole radiation associated with particles of arbitrary morphology using the discrete-dipole approximation (DDA) method. A paper on this work has appeared in Applied Optics, 45, 9115-9124, (2006).
- g) We have completed a study on the use of the finite-difference time-domain (FDTD) method to simulate the electromagnetic radiation emitted by an infinitesimal electric dipole embedded in a small particle with an arbitrary shape and internal composition. A paper on this work has appeared in JQSRT, 106, 257-261, (2007)
- h) We have completed a study of the light scattering by a small volume element filled with randomly positioned particles and were able to include the variation of the particles' positions in the far-field modified uncorrelated single-scattering approximation (MUSSA) which leads to the incoherent summation of the phase matrices of particles in the volume. A paper on this work has appeared in Optics Express, 15, 8479-8485. (2007).
- i) We have completed a study on the comparison of the surface and volume integration methods used in the FDTD formulation. A paper on this work has appeared in JQSRT, 106, 590-594, (2007)
- j) We have completed a very thorough study of the asymptotic light field in the ocean where we have included polarization as well as Raman scattering. A paper on this work is presently being prepared for publication in Applied Optics.

RESULTS

- a) The underwater polarized light field in a coupled atmosphere-ocean system goes to an asymptotic form in deep oceans, which means that the radiance and the degree of polarization become independent of the incident light field and become azimuthally-symmetric. Although the asymptotic radiance has been extensively studied, a comparison of the asymptotic nature of the radiance to that of the degree of polarization has not been performed. We simulated the underwater light field using a

vector radiative transfer model down to an optical depth of 100. Our results, as shown in Fig.1 below, implies that the radiance reaches its asymptotic form more quickly than the degree of polarization does. For the model used for the results presented we assumed a homogeneous water body with a single scattering albedo of 0.9, and the Petzold phase function was used for the hydrosols; however, the remaining part of the Mueller matrix was taken to be that for Rayleigh scattering. Here we use the zenith angle of the maximum value in the radiance pattern (θ_{rad}) and the zenith angle of the minimum value in the degree of polarization pattern (θ_{pol}) as indicators for the asymptotic regime. In shallow water, both θ_{rad} and θ_{pol} are determined by the refraction of the direct sunlight, while in the asymptotic region these angles move to 0

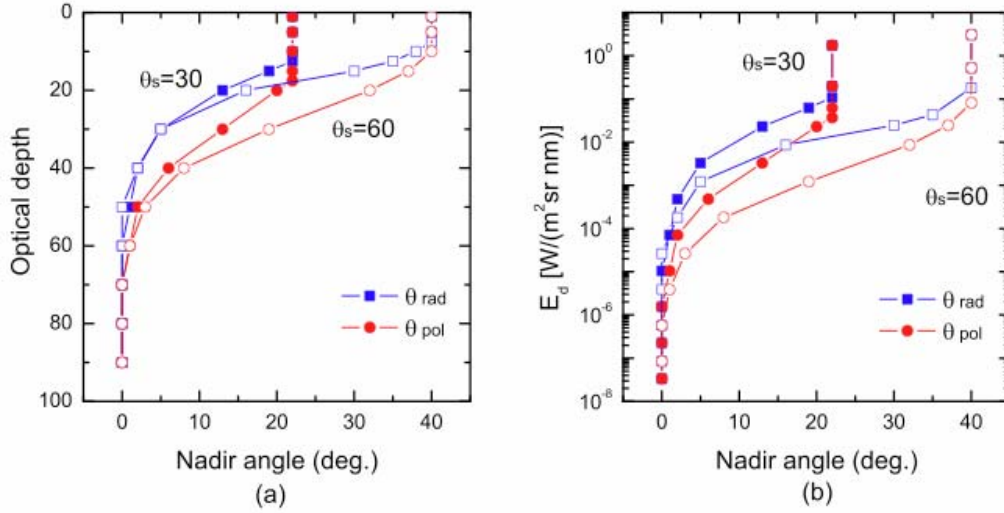


Figure 1. Movement of θ_{rad} and θ_{pol} as the optical depth increases and the downward plane irradiance decreases, in a coupled atmosphere-ocean system. The Petzold phase function was used for the ocean, and a single scattering albedo $\omega_0 = 0.9$ was assumed.

Results for two solar zenith angles $\theta_s = 30^\circ$ (curves with solid symbols) and $\theta_s = 60^\circ$ (curves with open symbols) are shown. This figure shows that the radiance (blue curves) reaches its asymptotic form more quickly than the degree of polarization (blue curves) does. The asymptotic region for the radiance is reached at optical depth of 60, while the asymptotic region for the degree of polarization is reached at optical depth of 70. The curve on the right shows the actual peak radiance relative to a $1 \text{ W}/(\text{m}^2 \text{nm})$ source at the top of the atmosphere

b) The comparisons between the results for the Platonic solids and four types of spherical equivalence show that the equal-surface-area spherical equivalence has the smallest errors in terms of the extinction cross section at both wavelengths. At a wavelength of $0.66 \mu\text{m}$, all the spherical equivalences substantially overestimate the asymmetry factors of the Platonic solids; and in the case of strong absorption, they underestimate the single-scattering albedo. The comparisons also show that the spherical equivalences cannot be used to describe the spatial distribution of scattered intensity associated with a prismatic polyhedron.

c) We have shown that our new FIRTM-AD is applicable not only to the hyperspectral sensors, but also to the narrowband sensors in the thermal IR spectral region. It is also applicable for the remote sensing of cloud properties using bispectral narrowband satellite measurements in the thermal IR region (e.g., 8–12 μm) .

d) We have shown that light scattering by a small volume element filled with randomly positioned particles, the far-field modified uncorrelated single-scattering approximation (MUSSA) leads to the incoherent summation of the phase matrices of particles in the volume. Our analytical results show that the MUSSA does not require the distance between any pair of particles in the volume to be larger than what is required in the single-scattering approximation (SSA). Instead, it requires the dimension of the volume to be large compared to the incident wavelength. The new results also make the requirements of MUSSA easier to be met.

IMPACT/APPLICATION

Our new work on internal dipole radiation can be used as another tool to understand the morphology and optical properties of particles ranging from bioaerosols to cells. It will lead to a fundamental understanding of both Raman scattering and fluorescence.

Our newly developed fast infrared radiative transfer model (RT) using as a basis the adding–doubling principle, referred to as FIRTM-AD, will play a major role in developing algorithms for hyperspectral sensing of cloud properties.

TRANSITIONS

We are using a modified FDTD code to perform the first calculations for the complete Mueller matrix for certain species of phytoplankton.

We have extended our FDTD method to include both anisotropic permittivities and permeabilities and will be able to analyze the new cloaking theory to make objects invisible!

We are also assisting Dr. Wenying Su of the NASA Langley Research Center by using our Ocean Monte Carlo program to interpret some satellite images he is trying to understand.

We are working with Dr. Talbot Waterman of Yale University to adapt our results for deep water light fields to be useful to biological oceanographers.

RELATED PROJECTS

We have written a new Monte Carlo code to emulate the temporal response of a pulse in a newly designed integrating cavity. This work is carried out in collaboration with Dr. Ed Fry whose group is designing a new integrating cavity capable of making measurements in the near UV

We are also assisting Dr Marlan Scully, a member of the National Academy of Sciences, in the development of a technique called FASTCARS to remotely detect anthrax spores.

We are working on several projects with our colleague, Dr. Ping Yang in the atmospheric Sciences Department, on problems involving remote sensing from satellites.

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