Monte Carlo Simulation of Electromagnetic Wave Propagation in Dense Random Media with Dielectric Spheroids

Benjamin E. BARROWES†, Chi O. AO††, Fernando L. TEIXEIRAT(a), Jin A. KONG†, and Leung TSANG†††, Nonmembers

SUMMARY We study the electromagnetic wave propagation in three-dimensional (3-D) dense random discrete media containing dielectric spheroidal scatterers. We employ a Monte Carlo method in conjunction with the Method of Moments to solve the volume integral equation for the electric field. We calculate the effective permittivity of the random medium through a coherent-field approach and compare our results with a classical mixing formula. A parametric study on the dependence of the effective permittivity on particle elongation and fractional volume is included.

key words: electromagnetic wave propagation, Monte Carlo methods, random media, effective permittivity

1. Introduction

In applications related to the remote sensing of the environment, the characterization of the electromagnetic wave interaction with natural media is of great importance. Natural media (e.g., snow, ice, and soil) often consist of a large number of densely packed, electrically small discrete scatterers that are randomly distributed in some background host medium.

The “classical” approach to study random discrete scatterers involves hypotheses such as the consideration of tenuous and/or sparse media. In sparse media, discrete scatterers occupy only a small volume fraction (typically less than 5%). In tenuous media, the constitutive parameters of discrete scatterers differ only slightly from that of the background medium. Such hypotheses allow for the solution of the problem through the independent scattering assumption, which neglects coherent interactions between the particles. However, in dense nontenuous media, the independent scattering assumption is no longer valid [4], [5], [7]; hence the effects of multiple scattering and coherent wave mutual interactions must be taken into account. This is also true for media in which the scatterers occupy a low overall fractional volume but can be locally dense due to clustering properties (e.g., branches and leaves in vegetation canopies).

For such dense media, analytical wave theory and approximations such as Foldy’s approximation [6], the quasicrystalline approximation (QCA) [8]–[10], and the QCA with coherent potential (QCA-CP) [4], [8] are frequently employed. In QCA and QCA-CP, the pair distribution function, which constitutes a second-order spatial correlation among the scatterers, must be specified. Common approximations for the pair distribution function are the hole correction and the Percus-Yevick (PY) pair distribution function [4], [11]. The use of such analytical techniques is adequate in the study of problems presenting configurational symmetries, such as media composed only of spherical particles. In many practical cases of interest, however, the adherence to spherical geometries is not able to capture the essential physics of the problem [1], [2]. The need to incorporate nonspherical statistics into the analytical models makes such analytical treatments rather involved.

The alternative to deal with more complex problems in a systematic manner is to resort to numerical methods. In [1], the scattering problem involving dense dielectric scatterers is formulated using a volume integral equation, which may then be solved by the Method of Moments (MoM) [3]. This gives the complete solution for a given configuration of scatterers. For a random media problem, the positions and properties of the scatterers are determined for different realizations according to some prescribed statistics using the Monte Carlo method. The MoM solution is sought for each realization so that statistical averages of the quantities of interest (e.g., effective permittivity, absorption rates, extinction rates, and phase functions of co-polarization and cross-polarization) can be determined.

In this work, we use the Monte Carlo method to characterize the effective permittivity of dense dis-
cretic random media composed of three-dimensional spheroidal dielectric scatterers as a function of the fractional volume of scatterers, particle elongation, the electromagnetic size of the particle (ka), and particle permittivity (media contrast). This extends previous studies (e.g. [11]–[14],[16]) on the numerical calculation of effective permittivity which were limited to spherical studies (e.g.[11]–[14],[16]) on the numerical calculation of permittivity (media contrast). This extends previous studies (e.g. [11]–[14],[16]) on the numerical calculation of effective permittivity which were limited to spherical particles and/or two-dimensional scattering.

2. Formulation

In this section, we briefly describe the volume integral formulation and the Monte Carlo methods used in our work. More detailed exposition can be found in [1].

Consider an incident electric field \( \mathbf{E}_{inc}(\mathbf{r}) \) impinging on \( N \) randomly positioned and oriented dielectric prolate spheroids (see Fig. 1). The total electric field \( \mathbf{E}(\mathbf{r}) \) can be expressed in terms of a volume integral equation as

\[
\mathbf{E}(\mathbf{r}) = \mathbf{E}_{inc}(\mathbf{r}) + k^2 \sum_{j=1}^{N} \int_{V_j} d\mathbf{r}' g(\mathbf{r},\mathbf{r}') [\chi(\mathbf{r}') \mathbf{E}(\mathbf{r}')] - \sum_{j=1}^{N} \nabla \int_{V_j} d\mathbf{r}' \nabla' g(\mathbf{r},\mathbf{r}') \cdot [\chi(\mathbf{r}') \mathbf{E}(\mathbf{r}')] \tag{1}
\]

where \( k = \omega \sqrt{\mu \epsilon} \) is the background wavenumber and \( V_j \) is the volume of the spheroid \( j \). The Green’s function \( g(\mathbf{r},\mathbf{r}') \) and electric susceptibility \( \chi(\mathbf{r}') \) are given by

\[
g(\mathbf{r},\mathbf{r}') = \frac{\exp(ik|\mathbf{r} - \mathbf{r}'|)}{4\pi|\mathbf{r} - \mathbf{r}'|}
\]

\[
\chi(\mathbf{r}') = \frac{\epsilon_p(\mathbf{r}')}{\epsilon} - 1.
\]

with \( \epsilon_p \) being the permittivity inside the spheroid.

To solve Eq. (1) using MoM, we assume that the spheroids are electrically small and choose the electrostatic solution of the Laplace equation to form a set of \( N_b \) basis functions. In this paper, only the dipole basis functions are considered. The matrix equation that results for the internal field \( \mathbf{E}(\mathbf{r}) \) is solved iteratively using the biconjugate gradient stabilized method (Bi-CGSTAB). It should be pointed out that permittivities of the background medium and the spheroid must satisfy the conditions \( ka \ll 1 \) and \( k_p a \ll 1 \), where \( k_p = \omega \sqrt{\mu \epsilon_p} \), in order for the small scatterer assumption to be valid.

To obtain the average fields, a Monte Carlo simulation is performed by creating multiple realizations of media consisting of thousands of discrete spheroids with random positions and orientations contained within some test volume. The Metropolis shuffling process [17],[18] is used to generate the positions and orientations of a system of densely packed spheroids. Periodic boundary conditions [1] are employed for the test volume in order to minimize edge effects.

3. Characterization of Random Media

Generally speaking, the characterization of a random medium containing discrete scatterers can be studied from two different perspectives: the coherent and incoherent fields. The coherent scattered field is obtained by averaging the electric field solution over \( N_r \) realizations:

\[
\langle \mathbf{E}_s \rangle = \frac{1}{N_r} \sum_{\sigma=1}^{N_r} \mathbf{E}_s^\sigma \tag{2}
\]

The coherent field is closely related to the propagation characteristics of the random media. On the other hand, the scattering of the coherent wave away from its forward propagation direction is related to the incoherent field, which is defined as

\[
\mathcal{E}_s^\sigma = \mathbf{E}_s^\sigma - \langle \mathbf{E}_s \rangle \tag{3}
\]

where \( \sigma = 1, 2, \ldots, N_r \) is the realization index. The incoherent intensity is then given by

\[
\mathcal{I}_s = \frac{1}{N_r} \sum_{\sigma=1}^{N_r} |\mathcal{E}_s^\sigma|^2 \tag{4}
\]

The incoherent intensity can be used to obtain the extinction coefficient and phase functions that are used in radiative transfer (RT) theory [1]. In contrast to “conventional” RT theory, the extinction coefficient and phase functions obtained through the Monte Carlo simulations take into account of coherent multiple interactions among the scatterers.
In this paper, we focus on the characterization of the propagation properties of the random media. Thus the coherent field will be used to determine the effective propagation constant of the random medium (or equivalently the effective permittivity for a non-magnetic medium). In this “coherent-field approach,” the effective permittivity is obtained as the result of an inverse scattering problem. The coherent scattered fields from a collection of particles in a given finite test volume are compared to fields scattered from a homogeneous volume of the same size and shape. The permittivity of the homogeneous medium which yields scattered fields that best match the averaged scattered fields produced by the random media is considered to be the effective permittivity. This approach has the advantages of taking the size and shape of the test volume into account.

It has been used for spheres contained in a cubic volume using the Born approximation for scattering from the cube [16], for 2-D rectangular regions [14], and for spheres contained in spherical volumes using Mie theory for scattering from the sphere [15], [16]. In the following, we apply this method to obtain the effective permittivity ($\epsilon_{\text{eff}}$) of a dense discrete random medium containing many spheroids by comparing the coherent scattered fields from collections of spheroids contained in a spherical test volume (Fig.1) to Mie scattering from the same size homogeneous sphere with permittivity equal to $\epsilon_{\text{eff}}$. The bistatic radar cross section (RCS) will be used for the comparisons.

Let the incident electric field $E_{\text{inc}}(r)$ be a plane wave

$$E_{\text{inc}}(r) = y \exp(ikz)$$  \hspace{1cm} (5)

The radar cross section (RCS) for the random spheroid medium ($\sigma_{\text{ran}}$) with the electromagnetic wavelength set to unity is then

$$\sigma_{\text{ran}} = 4\pi r^2 |<E_s>|^2.$$  \hspace{1cm} (6)

The Mie scattering in the far field is computed using Wiscombe’s code [21]. According to the notation in [21], the RCS of a Mie sphere $\sigma_{\text{mie}}$ in the scattering plane is given by

$$\sigma_{\text{mie}} = \frac{4\pi}{k^2} |S_1(\theta)|^2$$  \hspace{1cm} (7)

where $S_1$ is the complex scattering amplitude, and $\theta$ is the scattering angle. The effective permittivity is calculated using a multistart Nelder-Mead simplex search method [19]. Only the real part of the effective permittivity is reported here. The error term used in this search method was chosen to be the absolute value of the cumulative difference between the spherical medium RCS, $\sigma_{\text{ran}}$, and the Mie sphere RCS, $\sigma_{\text{mie}}$:

$$\text{error} = \delta_{\sigma} = \sum_{j=1}^{N_u} |(\sigma_{\text{mie},j}) - (\sigma_{\text{ran},j})|.$$  \hspace{1cm} (8)

where $\sigma_{\text{mie},j}$ and $\sigma_{\text{ran},j}$ denote the RCS for the Mie sphere and the random spheroid medium respectively at the $j$th angle. $N_u$ represents the number of scattering angles used in the minimization process ($N_u=39$ for the results presented in this paper).

A cumulative logarithmic error was also considered. However, the resulting $\epsilon_{\text{eff}}$ was slightly unstable. Using a logarithmic fit, even changes in scattering amplitude on the order of $10^{-4}$ would alter the resulting fit due to the emphasis placed on all scattering point. When using the linear error, the strong forward scattered field is fit best, and the behaviour in the tails is accounted for automatically. In this paper, only the real part of $\epsilon_{\text{eff}}$ is considered.

4. Numerical Results

The effective permittivity, $\epsilon_{\text{eff}}$ of dense random media containing discrete prolate spheroids was calculated for many combinations of $f_v$ (fractional volume) and $e$ (elongation, $c = ae$). For each $\epsilon_{\text{eff}}$ calculation, $N_u=50$ realizations were performed, and the results averaged according to Eq. (2) to yield the coherent scattered electric field $<E_s>$. The spherical test volume was first generated as a cubic test volume in order to employ periodic boundary conditions. After placement, the center of each spheroid was used to determine whether or not that spheroid would remain in the spherical test volume. $N=3000$ spheroids were placed in the cubic test volume, and therefore an average of $(N\pi/6) \approx 1571$ spheroids remained in the spherical test volume. The radius of the equivalent homogeneous sphere ($R$) used for Mie scattering was determined by

$$R = \left( \frac{N}{f_v} \left( \frac{\pi}{6} \right) a^3 e \right)^{\frac{1}{2}}.$$  \hspace{1cm} (9)

The parameters for the simulations reported here were $f_v \Rightarrow [0.05, .10, .15, .20, .25, .30, .35, .40], e \Rightarrow [1.0, 1.8, 2.6], \epsilon_p \Rightarrow 3.2$, and $ka \Rightarrow 0.2$. Both the random spheroid medium scattering and the Mie sphere scattering were copolarized scattering with $\phi = 0^\circ$ and $\theta = 0^\circ$ to $180^\circ$. Typical scattering results for the case of $f_v=0.20$, $e=1.0$ (sphere case) and 2.6, $ka=0.2$, and $\epsilon_p=3.2+0.0i$ are shown in Fig. 2. As with previous results for spheres [16] and 2-D infinitely long cylinders [14], the coherent scattering from a homogeneous volume with permittivity $\epsilon_{\text{eff}}$ adequately model the coherent scattering from dense random media consisting of discrete spheroids.

The variation of $\epsilon_{\text{eff}}$ with $f_v$ and $e$ is depicted in Fig. 3. Also shown is the $\epsilon_{\text{eff}}$ predicted by the classical mixing theory for spheres (solid line) and for spheroids with $e=2.6$ (dash-dot line). The classical mixing formula for randomly oriented ellipsoids is expressed as

$$\epsilon_{\text{eff}} = \epsilon + \left( 1 - \frac{f_v}{3} \sum_{i=1}^{3} N_i \beta_i \right)^{-1} \frac{f_v}{3} \sum_{i=1}^{3} \epsilon \beta_i$$  \hspace{1cm} (10)
where
\[ \beta_i = \frac{(\epsilon_p - \epsilon)}{\epsilon + N_i(\epsilon_p - \epsilon)}. \] (11)

In the prolate spheroid case considered in this paper, the depolarization factors \( N_i \) are given by [22]
\[ N_z = \frac{1 - \varepsilon^2}{2\varepsilon^3} \left( \ln \frac{1 + \varepsilon}{1 - \varepsilon} - 2\varepsilon \right) \] (12)
\[ N_x = N_y = \frac{1}{2}(1 - N_z) \] (13)
with the eccentricity \( \varepsilon = \sqrt{1 - (1/e^2)} \).

For the case of a dense medium consisting of spheres (\( e=1 \)), the results for effective permittivity are in excellent agreement with the classical mixing formula except at higher fractional volumes where the results are slightly lower. For the case of a dense medium consisting of randomly oriented prolate spheroids (\( e=2.6 \)), the results for effective permittivity are lower than that predicted by the classical mixing formula at \( f_v \) larger than about 0.2. These results are consistent with [16] for the spherical case. Note that as the fractional volume increases, the close proximity of the spheroids might necessitate the use of quadrupole terms to accurately model multiple scattering.

When interpreting numerical simulation results, accuracy and convergence of the computational method are important. A convergence criteria of residual error \( \leq 10^{-6} \) was used in the iterative solver (Bi-CGSTAB) for Eq. (1). To ensure that the medium sample set was sufficiently random, many realizations were performed. Figure 4 shows the calculated \( \epsilon_{\text{eff}} \) and the final error term (Eq. (8)) resulting from the Nelder Mead simplex search as a function of the number of realizations performed. As the number of realizations increases the residual error decreases and \( \epsilon_{\text{eff}} \) converges to its final value.

Table 1 lists the real part of \( \epsilon_{\text{eff}} \) calculated from the method described in this paper. These results provide numerical validation for the classical mixing formula for fractional volumes in the range of 0.05 to 0.4 for spheroids with elongations up to 2.6.

5. Conclusions

In this work, the effective permittivity (\( \epsilon_{\text{eff}} \)) of dense random media was studied. The coherent scattered fields from a collection of particles in a given test volume were compared to fields scattered from a homogeneous volume of the same size and shape. The permittivity of the homogeneous medium which yielded scattered fields that best matched the averaged scattered fields produced by many configurations of particles was...
considered to be equal to $\epsilon_{\text{eff}}$.

The effective permittivity of dense random media containing discrete spheroids was characterized through a Monte Carlo simulation employing the Method of Moments on the volume integral equation. The basis functions were chosen to be the electrostatic dipole solutions of a spheroid. Simulations with $N_v=3000$ particles, $N_r=50$ realizations and different fractional volumes ($f_v=0.05–0.40$) and particle elongations ($e=1.0–2.6$) were performed in a spherical test volume. The scattering from this volume was then compared to Mie scattering from a homogeneous sphere of the same size. Results indicate that $\epsilon_{\text{eff}}$ for a dense random media containing randomly oriented discrete prolate spheroids agrees well with results from the classical mixing formula. This is consistent with previous studies considering spherical particles only.

Acknowledgement

This work was supported by National Science Foundation (NSF) under grant numbers ECS9615799 and ECS9423861, by the Office of Naval Research (ONR) under contract numbers N00014-99-1-0175 and N00014-97-1-0172, and through a NSF Graduate Fellowship.

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References


\[ \text{Benjamin E. Barrowes} \] received his B.S. and M.S. degrees in Electrical Engineering from Brigham Young University both in 1999. He is currently pursuing the Ph.D. degree in Electrical Engineering from the Massachusetts Institute of Technology, Cambridge. His research interests include wind-wave interaction, electromagnetic wave scattering from the sea surface and from random media.

\[ \text{Chi O. Ao} \] received his A.B. degree in physics from the University of California at Berkeley in 1993. He is currently pursuing his Ph.D. at the Massachusetts Institute of Technology. His research interests include theoretical and numerical studies of electromagnetic wave scattering in random media and rough surfaces.

\[ \text{Fernando L. Teixeira} \] received the B.S. and M.S. degrees in electrical engineering from the Pontifical Catholic University of Rio de Janeiro (PUC-Rio), Rio de Janeiro, Brazil, in 1991 and 1995, respectively, and Ph.D. degree in electrical engineering from the University of Illinois at Urbana-Champaign in 1999. Currently, he is a post-doctoral fellow at the Center for Electromagnetics Research and Applications at MIT.

\[ \text{Jin A. Kong} \] is a Professor of electrical engineering at the Massachusetts Institute of Technology (MIT), Cambridge. He has published eight books, including *Electromagnetic Wave Theory* (New York: Wiley, 1990), more than 400 refereed articles and book chapters, and supervised more than 120 theses. He is Editor-in-Chief of the *Journal of Electromagnetic Waves and Applications*, Chief Editor of the book series *Progress in Electromagnetics Research*, and Editor of the Wiley Series in *Remote Sensing*. His research interests include electromagnetic wave theory and applications.

\[ \text{Leung Tsang} \] received the B.S., M.S., and Ph.D. degrees from the Massachusetts Institute of Technology (MIT), Cambridge, in 1971, 1973, and 1976, respectively. He has been a Professor of electrical engineering at the University of Washington, Seattle, since 1986. He is coauthor of the book *Theory of Microwave Remote Sensing* (New York: Wiley, 1985). His current research interests include remote sensing, wave propagation in random media and rough surfaces, and optoelectronics. Dr. Tsang is a Fellow of the Optical Society of America. He was the Technical Program Chairman of the 1994 IEEE Antennas and Propagation International Symposium and the Technical Program Chairman of the 1995 Progress in Electromagnetics Research Symposium in Seattle. Since 1996, he has been the Editor-in-Chief of the *IEEE Transactions on Geoscience and Remote Sensing*. 