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Direct simulation of extinction in a slab of spherical particles

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ABSTRACT

The exact multiple sphere superposition method is used to calculate the coherent and incoherent contributions to the ensemble-averaged electric field amplitude and Poynting vector in systems of randomly positioned nonabsorbing spherical particles. The target systems consist of cylindrical volumes, with radius several times larger than length, containing spheres with positional configurations generated by a Monte Carlo sampling method. Spatially dependent values for coherent electric field amplitude, coherent energy flux, and diffuse energy flux, are calculated by averaging of exact local field and flux values over multiple configurations and over spatially independent directions for fixed target geometry, sphere properties, and sphere volume fraction. Our results reveal exponential attenuation of the coherent field and the coherent energy flux inside the particulate layer and thereby further corroborate the general methodology of the microphysical radiative transfer theory. An effective medium model based on plane wave transmission and reflection by a plane layer is used to model the dependence of the coherent electric field on particle packing density. The effective attenuation coefficient of the random medium, computed from the direct simulations, is found to agree closely with effective medium theories and with measurements. In addition, the simulation results reveal the presence of a counter-propagating component to the coherent field, which arises due to the internal reflection of the main coherent field component by the target boundary. The characteristics of the diffuse flux are compared to, and found to be consistent with, a model based on the diffusion approximation of the radiative transfer theory.

1. Introduction

Modern, parallel-based computational hardware, coupled with superposition methods for calculating the net scattered field by a collection of particles, have made feasible the use of direct simulation strategies to investigate the characteristics of electromagnetic energy transport in dense particulate systems. A direct simulation, by definition, provides an exact description of the electromagnetic field both within and external to a target containing a large yet finite number of particles, and which is excited by an external source of radiation. In this sense, results generated by direct simulations can be considered a benchmark for evaluation of analytical or phenomenological theories to describe the propagation of electromagnetic energy in discretely inhomogeneous media. As a case in point, we have recently used the multiple sphere T matrix (MSTM) code to calculate the scattering matrices of targets containing up to several thousand spheres, with the individual spheres having size parameters up to 4 [1–3]. The targets, in these calculations, consisted of spherical volumes, with the spheres randomly distributed within the volume with a set overall

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volume fraction; volume fractions used in the calculations ranged from 0.01 to 0.4. Since the number of spheres in the targets was large, we assumed that the configuration-averaged scattering matrix (i.e., that obtained from averaging scattering matrices, each obtained for a fixed realization of the sphere properties and a fixed incident direction) could be approximated by the orientation averaged scattering matrix for a single realization; this allowed us to exploit the analytical orientation averaging properties of the target *T* matrix as calculated by MSTM. Results from these calculations have provided definitive evidence to support microphysical theories of radiative transfer and coherent backscattering [4].

The objective of this work is to present a similar comparison between numerically exact computer simulations and analytical theory. The phenomena under examination, in this case, are the attenuation of the coherent field, and the propagation of the coherent and diffuse components to the time-averaged Poynting vector in a particulate medium, due to scattering by the particles. The simulation procedure is relatively straightforward: local electric and magnetic field amplitudes will be calculated for a statistically representative sequence of randomly generated targets of spheres, with each target configuration corresponding to the same sphere properties and average concentration. The local coherent field and time-averaged Poynting vector are then obtained by assuming ergodicity and averaging over the sequence of configurations. An important difference in the procedures used here, as opposed to our previous investigations [2,3], is that they will not employ analytical *T* matrix averaging: our focus is on the local field amplitudes within the medium as opposed to the far-field scattering behavior.

A well established theoretical framework has been developed to describe coherent field attenuation in discretely inhomogeneous media. On the most basic level is the standard radiative transfer theory, which represents the dilute concentration limit [2,4]. The imaginary part of the effective propagation constant in the medium, for this approximation, is obtained from the product of the particle number density and average extinction cross section.

The radiative transfer theory is based on the far-field version of the Foldy–Lax equations [4] and will fail for wavelength-sized particles with concentrations approaching and exceeding 0.1. For such cases comprehensive effective medium (EM) formulations have been developed, most notably by Ishimaru and the Varadans [5–7]. Such theories begin with the same basic superposition model employed in the direct simulation, for which the exciting field at a particular sphere is given by the incident (i.e., externally exciting) field and the sum of fields scattered from every other sphere in the system. Unlike a direct simulation – which solves the superposition equations for each sphere in the system and then averages over multiple configurations – EM formulations attempt to average the superposition equations analytically, with subsequent derivation of relations for the effective propagation constant. Performing this averaging requires knowledge of the pair correlation function of the particles in the random medium, and it also invokes simplifying assumptions regarding the high-order correlations among the particle positions and scattered fields, e.g., the quasi-crystalline approximation (QCA) [8–10].

Both computational and experimental evidence has been collected to validate EM theories. Tsang et al. [11] inferred the attenuation rate from direct simulations of far-field scattering by a particulate volume and obtained good correspondence with theory, although the simulations were limited to spheres with a relatively small size parameter of 0.2. Analytical estimates of EM theories have been shown to accurately predict laboratory measurements of extinction in random suspensions of monodisperse spheres having size parameters of order unity or greater [12].

The investigations in [11,12] were focussed entirely on the effective propagation constant (or, equivalently, effective refractive index) of the spherical-particle system. As predicted by theory, this quantity depends solely on the sphere properties, concentration, and pair correlation function; it is not a function of the geometry of the system containing the particles. Unlike Ref. [11], the objective of this work is to examine how the target geometry affects the coherent field within the target. In particular, we will employ targets which model a fixed-thickness slab of particles. In an EM model, such a system would represent a plane layer. It is well known that interference of the forward and backward-propagating plane waves in a homogeneous plane layer can strongly affect the reflectance and transmission of the layer. We will show that the coherent field, in a slab of random spherical particles, can also cause interference effects.

An additional objective of this work is to examine the character of electromagnetic energy transport in the random medium. In particular, the direct simulations, combined with configurational averaging, will be used to calculate the coherent and diffusive components to the time-averaged Poynting vector in the medium. We will apply the diffusion approximation of the radiative transfer theory to model the diffuse flux.

2. Methodology

2.1. Basic definitions

We assume that the time dependence of the electric and magnetic fields is harmonic and described, in the complex-field representation, by the simple complex exponential $\exp(-\mathrm{i}\omega t)$, where ω is the angular frequency, t is time, and $\mathrm{i}=\sqrt{-1}$. In other words, we assume that the complex electric and magnetic fields can be factorized as $\mathbf{E}(\mathbf{r},t)=\exp(-\mathrm{i}\omega t)\mathbf{E}(\mathbf{r})$ and $\mathbf{H}(\mathbf{r},t)=\exp(-\mathrm{i}\omega t)\mathbf{H}(\mathbf{r})$ respectively, where $\mathbf{r}$ is the position (radius) vector, while the actual real-valued fields are obtained by talking the real part of the respective complex fields. The complex field amplitudes $\mathbf{E}(\mathbf{r})$ and $\mathbf{H}(\mathbf{r})$ are constant if the scattering target is fixed, but vary with time implicitly if the scattering object undergoes temporal changes. In what follows, we will assume that temporal fluctuations of $\mathbf{E}(\mathbf{r})$ and $\mathbf{H}(\mathbf{r})$ caused by changes in the scattering object occur much more slowly than the harmonic oscillations of the factor $\exp(-\mathrm{i}\omega t)$.