Evaluation of Effective Electrical Properties for Lossy Periodic Composite Structures Using a Finite Difference Method

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Abstract

In this paper, we introduce a three-dimensional numerical procedure to evaluate frequency-dependent and anisotropic electrical properties of arbitrary three-dimensional mixtures/formations. Only a unit element is required in the modeling. The numerical technique is based on a periodic three-dimensional finite-difference method. Several numerical examples are used to demonstrate effectiveness of this method. It is shown that this method can be applied to characterize medium heterogeneous properties for mixtures with anisotropies in both mixture geometries and medium electrical properties

1. Introduction

Over the last century, research in diverse fields has been performed to understand physical properties of heterogeneous mixtures. In general, mixtures consisting of different materials or the same materials in different states have often been explored. The electrical properties, including permittivity and conductivity, of a material are fundamental properties, which are required for various applications in geophysical mapping, remote sensing, medical research, materials science, and non-destructive testing. However, it is still a challenging task to characterize these properties of composite materials since actual composite media are extremely complex and inclusions are at multiple length scales. Due to the fact that the length scales of such composite components can range over several different orders, observation of the heterogeneity is often restricted by any dimension of the considered sample. The size, shape, spatial arrangement, and interactions between the different constituents of the material medium are the key to their extraordinary properties. To study the details of this complex system and its relation to the properties of materials, both analytical and numerical methods are proposed. Among the available analytical methods, Maxwell-Garrent and Bruggeman formulas [1], which are based on the conventional mixing-law theory, have served as the fundamentals for these techniques. Although improved analytical approaches are computationally efficient, they can only be applied to evaluate complex composite materials with limited shapes of inclusion at low volume fractions. With the rapid development of computational electromagnetics as well as computer hardware, various numerical methods have been proposed and are widely used currently. These numerical methods can be applied to arbitrary shapes of inclusions at very high volume fractions.

The purpose of this thesis is to develop an efficient numerical technique to study the relationship between the micro-scale inclusion and macro-scale mixture electrical properties. The method is based on a simple finite difference method at low frequency regions. The proposed method can be applied to evaluate the effective permittivity of arbitrary composite structures containing dispersive materials. Several interesting results of extremely distinctive inclusions are obtained via this developed method and compared with the single pole Debye model [2].

2. Methodology

It is observed that many composite formations/mixtures, especially those encountered in geophysical and electromagnetic applications, often consist of periodic arrangement of unit elements whose dimensions are much smaller than the operating wavelength. Therefore, in our studies, we assume that composite structures are periodic in all three directions, as shown in Fig. 2-1.

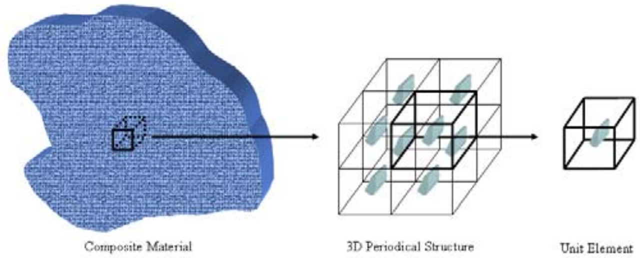


Figure 1. Unit element definition.

Since periodicity of composite unit element is typically smaller than the operating wavelength, the quasi-static simplification is used in this study. Under this assumption, the electric potential inside mixtures are governed by the Laplace's equation, given by $\oiint_S (\varepsilon \nabla \phi) \cdot ds = 0$,where ϕ and ε are the electric potential and the medium permittivity. Instead of using real medium permittivity, the complex permittivity is adopted here $\hat{\varepsilon} = \varepsilon + {i\sigma}/{\omega}$. For homogeneous medium, the system equation becomes

$$\begin{aligned}
&\varepsilon_x^{i,j,k} \frac{\phi_{i+1,j,k} - \phi_{i,j,k}}{dx^2} + \varepsilon_y^{i,j,k} \frac{\phi_{i,j+1,k} - \phi_{i,j,k}}{dy^2} \\
&+\varepsilon_z^{i,j,k} \frac{\phi_{i,j,k+1} - \phi_{i,j,k}}{dz^2} - \varepsilon_x^{i-1,j,k} \frac{\phi_{i,j,k} - \phi_{i-1,j,k}}{dx^2} \\
&-\varepsilon_y^{i,j-1,k} \frac{\phi_{i,j,k} - \phi_{i,j-1,k}}{dy^2} - \varepsilon_z^{i,j,k-1} \frac{\phi_{i,j,k} - \phi_{i,j,k-1}}{dz^2} = 0,
\end{aligned} \tag{1}$$

where $\varepsilon_x^{i,j,k}, \varepsilon_y^{i,j,k}, \varepsilon_z^{i,j,k}$ are the complex effective *x-, y-* and *z*-directional permittivities defined at the edges of the element cell (*i, j, k*).

With the assumption that mixtures have periodic patterns in one or more dimension, the evaluation of mixture effective medium permittivities can be performed within one unit element with proper boundary conditions and source excitation. For instance, to evaluate the *z*-directional permittivity of a mixture, the required periodic boundary conditions and external voltage source are given by,

$$\begin{aligned}
&\phi(X_{\max}, j, k) = \phi(0, j, k), \\
&\phi(i, Y_{\max}, k) = \phi(i, 0, k), \\
&\phi(i, j, Z_{\max}) = \phi(i, j, 0) + V,
\end{aligned} \tag{2}$$

where $X_{\max}$, $Y_{\max}$, and $Z_{\max}$ are numbers of grid in the finite difference method along the *x*, *y*, and *z* directions, respectively. *i, j*, and *k* are lattice locations as defined previously.

After solving equations (1) and (2) by using the FDM, the internal electric potentials and corresponding electric fields can be obtained. Consequently, the *z*-directional permittivity can be computed as follows:

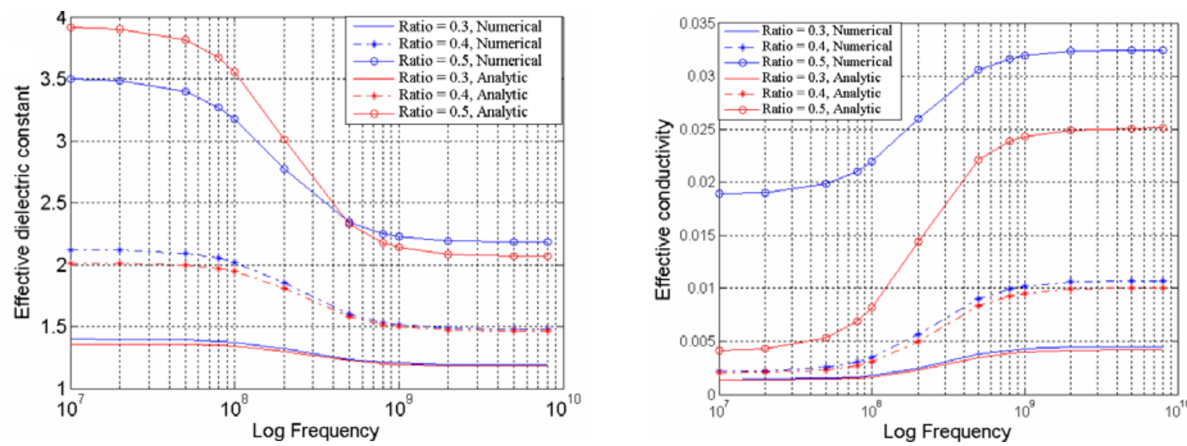
$$\begin{aligned}
\varepsilon_z^{eff} &= \frac{(dz \cdot Z_{\max})}{(dx \cdot X_{\max}) \cdot (dy \cdot Y_{\max})} \frac{Q}{V} \\
&= \frac{(dz \cdot Z_{\max})}{(dx \cdot X_{\max}) \cdot (dy \cdot Y_{\max})} \frac{\int_{surface} D \cdot ds}{V} \\
&= \frac{(dz \cdot Z_{\max}) \cdot \int_S \varepsilon_z(i,j,Z_{\max}) \frac{\phi(i,j,Z_{\max}) - \phi(i,j,Z_{\max-1})}{dz} ds}{V \cdot (dx \cdot X_{\max}) \cdot (dy \cdot Y_{\max})}
\end{aligned} \tag{3}$$

.

It is noted that equation (3) is different from the formulation used by Karkkainen [3], where only isotropic properties can be extracted. Equation (3) can be used to evaluate the effective medium parameters for anisotropic medium. Following the aforementioned procedure, the effective permittivies along the other two directions can be obtained by interchanging the direction of voltage source and periodic boundary conditions. In other words, three simulations are required to extract the effective permittivities for dielectric mixtures with biaxial anisotropic inclusions [4].

3. Numerical Examples

To examine the frequency-dependent behavior of mixtures [5-7], conductive losses are introduced into the mixtures. For the purpose of validating our approach, a spherical inclusion inside a cubic host medium is examine. Instead of lossless media, lossy media example is specified by the host conductivity of 0.001 S/m and inclusion conductivity of 0.1 S/m. Besides, the relative permittivity is 1.0 for the host medium 4.0 for the inclusion, respectively. Figs 2(a) and 2(b) showed the extracted permittivity and conductivity of this mixture as a function of frequency at three different volume fractions. The ratio in the figures is defined as the radius of the spherical inclusion to that of the cubic host edge length. It is observed that when this value is smaller than 0.4, the analytical results agree well with the numerical solutions. However, as this ratio increases, large discrepancies in both permittivity and conductivity are observed in both figures. It is believed that such discrepancies are caused by the inaccuracy of the analytical solution for large volume mixture electrical property characterization. Since the larger ratio leads the higher volume fraction, the disparities of the results with ratio equal to 0.5 in the figures are predicted.



(a) (b)

Figure 2. Effective (a) dielectric constant and (b) conductivity of a spherical inclusion with three different radiuses inside a cubic host.

Most physical materials can be described with the single-pole Debye equation given by

$$\hat{\varepsilon}_r(\omega) = \varepsilon_\infty + \frac{\varepsilon_s - \varepsilon_\infty}{1 + j\omega\tau} - \frac{j\sigma_e}{\omega\varepsilon_0} \quad . \tag{4}$$

Equation (4) adds one more term into the original Debye model to consider the conductivity loss in dispersive material, where σ_e is the D.C. electric conductivity of the material and ε_0 is the permittivity of free space. In order to compare the numerical results with this single-pole Debye model, the first lossy medium example, a spherical inclusion inside a cubic host, is explored again. To see the relationship between all the parameters of equation (4) and the inclusion volume, a variable *R*, defined by the ratio between the radius of the spherical inclusion and the edge length of the cubic host, is used to adjust the volume fraction as the following figures. Figs. 3(a) to 3(b) are the comparisons between the numerical results of five different inclusion radiuses (between *R* =0.1 and *R* =0.5) and the fitting results of single-pole Debye model. As plotted in those figures, the numerical results of our proposed method match very well with the single-pole Debye model.

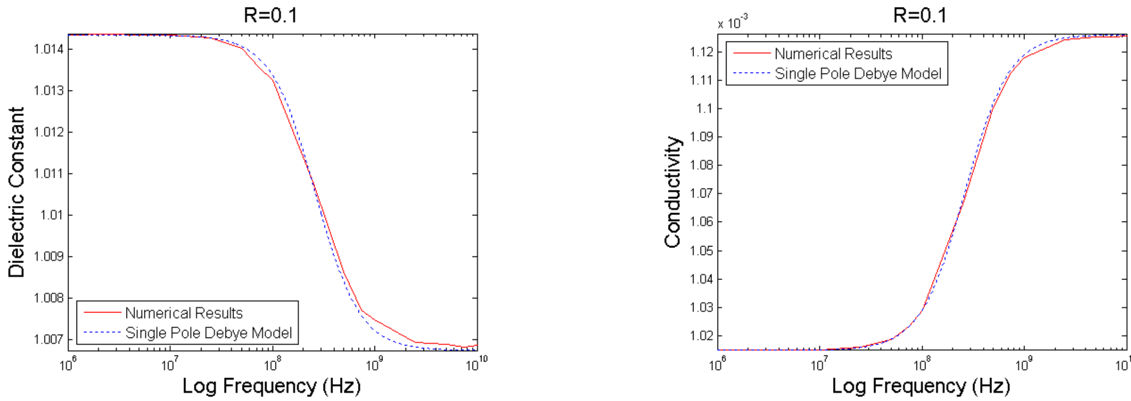


Figure 3. Comparison between single-pole Debye model and numerical results of effective electrical properties ((a)dielectric constant and (b) conductivity) with R=0.1.

4. Conclusion

A three-dimensional finite difference method was developed in this thesis to evaluate anisotropic dielectric properties of composites with non-symmetric geometries and/or biaxial anisotropic material properties. The simulation results showed that this proposed numerical method is a versatile numerical approach to estimate the anisotropic dielectric properties of complex dielectric mixtures. Using this approach, examples of inclusions with material anisotropicity and geometrical anisotropicity were investigated.

5. References

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