Numerical Modelling of Dielectric Mixtures

Antoniya R. Georgieva

Abstract - **The present paper reports the results of a numerical analysis of electromagnetic fields in two component dielectric mixtures. The mixture consists of a homogeneous background in which circular cylinders are embedded. Both materials are lossless. Finite-difference time-domain method is used to simulate wave propagation through the mixture. The effective permittivity is determined from the reflection coefficient. The numerical results are compared with theoretical mixture models.**

Keywords - **Dielectric mixture, artificial dielectric, effective permittivity, FDTD method.**

I. INTRODUCTION

Materials encountered in nature are quite often inhomogeneous and complicated in structure. Many of them, like snow, sea ice and soil, consist of several phases with different electromagnetic properties. Such media are referred as dielectric mixtures in literature. One of the phases is usually considered as a background medium and the other are treated as inclusions.

The problem of interaction between electromagnetic waves and such a complex material object is quite a difficult one to solve. However, under certain conditions the dielectric mixture could be considered as a homogeneous medium characterized by only one macroscopic parameter - the effective permittivity (the components of the mixture are assumed non-magnetic).

The properties of dielectric mixtures depend on the internal structure of the medium i.e. the shape, the volume fraction, and the arrangement of the different components. This makes it possible to develop new artificial materials having desired electromagnetic properties.

The history of the study of heterogeneous mixtures dates back to 19th century and several analytical and empirical models have been proposed. The advances in computer technology in the recent years made it feasible to perform numerical predictions for the electrical parameters of mixtures.

This paper demonstrates an approach for determining the characteristics of a heterogeneous lossless two-phase mixtures numerically by means of the Finite Difference Time Domain (FDTD) method. This is a dynamic method to solve the full set of Maxwell equations in a finite region. For computational restrictions, a two-dimensional mixture is treated instead of the full three-dimensional case. The inclusions are two-dimensional spheres (cylinders). Both regular lattice and random location of inclusions are studied.

The effective permittivity of the material is deduced from the reflection coefficient at the surface of the mixture by transmission line analogy. The effective permittivity concept is defined to the permittivity of such a homogeneous sample from which the reflection coefficient is the same as from the mixture under study. The simulation is carried out in free space.

The results are obtained as a function of the volume fraction (the volume of inclusions to volume of background medium ratio) for various contrasts between permittivities of the ingredients.

The numerical results are compared to the most common mixing rule predictions such as the Maxwell-Garnett and Bruggeman models.

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II. MIXING FORMULAS IN TWO DIMENSIONS

As mentioned previously, the attention in the following is limited to 2-D mixtures. In the literature, many mixing models can be found for the effective dielectric permittivity of mixtures. The major limitation of this models is that the inhomogeneities have to be of clearly smaller scale than the wavelength of the operating field. Otherwise scattering effects inside the medium cannot be neglected and the concept of the effective permittivity loses its physical meaning. Here are presented some of the commonest mixing formulas.

The oldest known mixing rule, the Maxell-Garnett formula, reads in two dimensions [2]:

$$\varepsilon_{eff} = \varepsilon_h + 2f\varepsilon_h \frac{\varepsilon_i - \varepsilon_h}{\varepsilon_i + \varepsilon_h - f(\varepsilon_i - \varepsilon_h)}, \qquad (1)$$

where circular inclusions (2-D spheres) of permittivity ε_i are embedded in homogeneous host medium (ε_h) and occupy a volume fraction f. It is to be noted that all permittivities in this paper are relative quantities.

Another famous mixing rule is the symmetric Bruggeman formula [2]:

$$(1-f)\frac{\varepsilon_h - \varepsilon_{eff}}{\varepsilon_h + \varepsilon_{eff}} + f\frac{\varepsilon_i - \varepsilon_{eff}}{\varepsilon_i + \varepsilon_{eff}} = 0. \qquad (2)$$

The approach presented in [2] collects dielectric mixing formulas in two dimensions into one family:

$$\frac{\varepsilon_{eff} - \varepsilon_h}{\varepsilon_{eff} + \varepsilon_h + v(\varepsilon_{eff} - \varepsilon_h)} = f\frac{\varepsilon_i - \varepsilon_h}{\varepsilon_i + \varepsilon_h + v(\varepsilon_{eff} - \varepsilon_h)}. \qquad (3)$$

For different values of the dimensionless parameter v, the previous mixing rules are recovered: $v = 0$ gives the Maxwell-Garnett rule, $v = 1$ gives the Bruggeman formula. The third approximation for $v = 2$ gives the Coherent Potential formula [2] known in solid state physics.

Different mixing models predict different effective permittivity values for a given mixture. However, there are theoretical bounds that limit the range of predictions. The loosest bounds are the so-called Wiener bounds [1,2]:

$$\varepsilon_{eff,\min} = \frac{\varepsilon_i \varepsilon_h}{f\varepsilon_h + (1-f)\varepsilon_i} \tag{4}$$

and

$$\varepsilon_{eff,\max} = f\varepsilon_i + (1-f)\varepsilon_h . \tag{5}$$

These two cases correspond to capacitors connected in parallel or series in a circuit. The bounds retain the minimum and maximum character independently of the type of the mixture, i.e. they are valid for both $\varepsilon_i > \varepsilon_h$ and $\varepsilon_i < \varepsilon_h$.

III. Principle of Numerical Calculation

The effective permittivity of a mixture is determined by calculation of the reflection coefficient from a sample. Both cases of a regular lattice and random positioned circular inclusions are studied. In the latter case overlapping of inclusions is allowed. The volume fraction of inclusions is controlled with their number keeping the radius constant.

Using a standard FDTD scheme [5], reflection from a sample of the mixture is simulated in free space. A case of parallel polarization is studied. The incident wave is a plain wave with components E_y and H_z coming from free space at an angle of 90^o to the sample surface. First order Mur's absorbing boundary conditions (ABC) are used to simulate infinite space outside the artificial computation domain borders. Fig.1 illustrates the simulation setup.

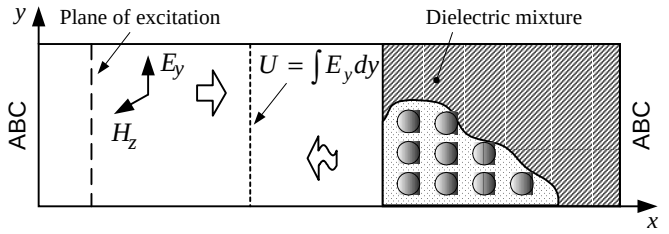

Fig.1. Schematics of the simulation setup. The dielectric mixture is formed of circular inclusions infinite in z-direction (cylinders). A plane wave is launched to travel in x-direction and reflection is studied. Electric field integrals are calculated in y-direction for each value of x to yield voltages.

The computational domain has a size of 150x50 cells. The used cell size is $\Delta x = \Delta y = 3$mm. The reflecting surface of the mixture is placed at $x = 65$. The diameter of inclusions is 6 cells. Excitation is performed at a distance of $10\Delta x$ from the left border of the computational domain. The time behavior of the excitation is a sinusoide of unit amplitude. One simulation is run as long as is needed to create a steady state.

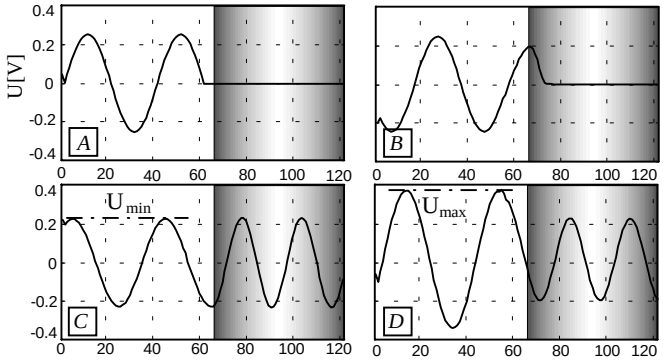

Fig.2. Reflection from dielectric mixture surface. Voltage is plotted as a function of x-coordinate, shown in spatial steps (one steps is equal to 3 mm). In A only the incident wave is shown, in B reflection starts, C and D show field pulses in time. Simulation is carried out at 1.5 GHz. The effective permittivity of the mixture is 2.4.

As results of the simulation, electric field integrals in y-direction are calculated for each time step. Each integral is equivalent to voltage between points with coordinates (x,0) and (x,50). The total field in front of the reflecting surface pulses, varying from a minimum ($U_{\min}$) to a maximum ($U_{\max}$) value as shown on Fig.2. The ratio of these values gives a voltage standing wave ratio (VSWR) defined by analogy with the transmission line theory:

$$VSWR = \frac{U_{\max}}{U_{\min}} = \frac{1+|R|}{1-|R|}.$$

where R is the reflection coefficient.

On the other hand the reflection coefficient can be determined from the Freshnel formulas. In the case of perpendicular incidence and parallel polarization we have:

$$R = \frac{1-\sqrt{\varepsilon_{eff}}}{1+\sqrt{\varepsilon_{eff}}} \quad \text{and} \quad |R| = \frac{\sqrt{\varepsilon_{eff}}-1}{\sqrt{\varepsilon_{eff}}+1}. \tag{7}$$

Substitution of (7) in (6) gives:

$$VSWR = \sqrt{\varepsilon_{eff}} . \tag{8}$$

Thus, the effective relative permittivity can be estimated by observing the total field variations in time in front of the reflecting surface.

An important issue in the simulation setup is incorporation of circular inclusions to the Cartesian square grid used for FDTD formulation of the Maxwell equations. Usually staircasing is used to represent curved boundaries provided that the grid cell is sufficiently smaller than the curved body. This technique, however, inevitably affects the accuracy of the simulation. To decrease this effect, in the current analysis weight coefficients are used for determining permittivity values between E field nodes when one of the nodes is inside an inclusion and the other lies in the background medium.

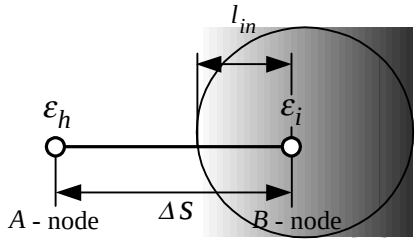

Fig.3. An estimation of the permittivity between two nodes lying in different media is based on geometry considerations.

Fig.3 illustrates this idea. The value of permittivity between the nodes "*A*" and "*B*" is:

$$\varepsilon_{A+B} = \frac{l_{in}}{\Delta s}\varepsilon_i + \frac{\Delta s - l_{in}}{\Delta s}\varepsilon_h , \qquad (9)$$

where l_{in} is the length of the cell edge part falling outside the inclusion boundary and Δs is the spatial step.

IV. Simulation Accuracy

The accuracy of the FDTD simulation can naturally be increased by decreasing the grid size (the spatial step). However, halving the cell size causes the computational time to grow by factor of four, and simulation must be run twice as long as before in terms on time steps.

A general rule in FDTD algorithm is to keep the spatial step much smaller (at least 20 times) than the shortest wavelength in the computational region [1]. At a frequency of 1,5 GHz within a region with maximum permittivity value of 10, the wavelength is 63 mm which is approximately 20 times larger than the grid size of 3 mm used in the simulation.

To test the influence of the grid size on the effective permittivity result, a number of simulation were performed in which inclusions were arranged in a regular lattice and their volume fraction was kept the same, but the cell size was varied. For mixtures with $\varepsilon_i < \varepsilon_h$ the results do not vary with the cell size. The composites with $\varepsilon_i > \varepsilon_h$, however, exhibit a slightly increasing trend in obtained permittivity value vs. cell size. Hence, for this type of mixture it is reasonable to use a denser grid.

The frequency of the simulation does not influence significantly the obtained effective permittivity. Simulations are carried out at three frequencies (700 MHz, 1 GHz and 1,5 GHz) and averaging is used to obtain a representative result.

V. Results

Effective permittivity was calculated for two types of mixtures - normal ($\varepsilon_i > \varepsilon_h$) and inverted ($\varepsilon_i < \varepsilon_h$). Both regular lattice and random distribution of inclusions are studied. Fig.4 illustrates field distribution inside such samples, detected at very low frequency (static case). There, contour plots of the electric field amplitude are given. Dark color corresponds to high values of electric field intensity. Light coloring marks the regions with low intensity values. The position of inclusions

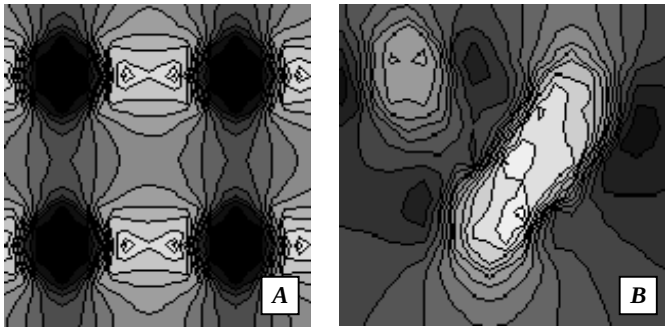

Fig.4. Electric field distribution in normal *(A)* and inverted *(B)* mixtures. In *A* a sample with regular lattice of inclusions is shown. In *B* the inclusions are randomly distributed. There are four inclusions, three of them are overlapping.

can be clearly seen. As expected, the field amplitudes are smaller in areas with higher dielectric permittivity.

The results for a medium with a regular lattice of inclusions are shown in Fig.5. The inclusion permittivity is ε_i = 2.5 and the host material is air (ε_h = 1). The cross sign denotes numerical results. Three analytical models are plotted too for volume fractions up to 1. However, the maximum volume fraction that could be achieved for regular lattice of inclusions is 0.78 (cylinders that do not overlap cannot fill the entire space).

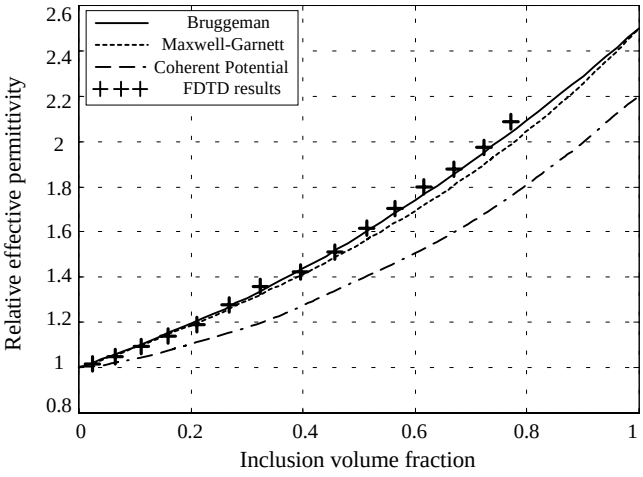

Fig.5. Effective permittivity of a mixture with $\varepsilon_i = 2.5$ and $\varepsilon_h = 1$ compared with theoretical models.

For low volume fractions the analytical results obtained from different formulas do not differ significantly. They all well coincide with numerical results. For high volume fractions Bruggeman model appears to be closest to the numerical results.

Fig.6 shows the results for inverted mixture with ε_i =1 and ε_h = 2.5 Comparison with Fig.5 shows that the results for a chosen volume fraction are not equal as Bruggeman symmetric formula predicts. Increasing of volume fraction and/or the difference between ε_i and ε_h causes this effect to become more significant.

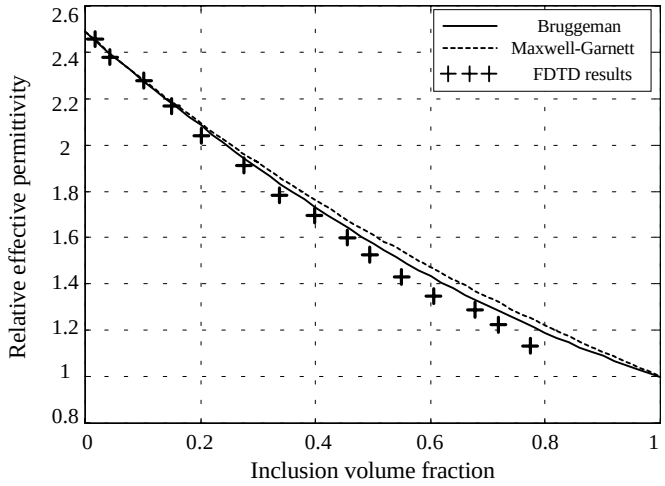

Fig.6. Effective permittivity of a mixture with $\varepsilon_i = 1$ and ε_h=2.5 compared with theoretical models.

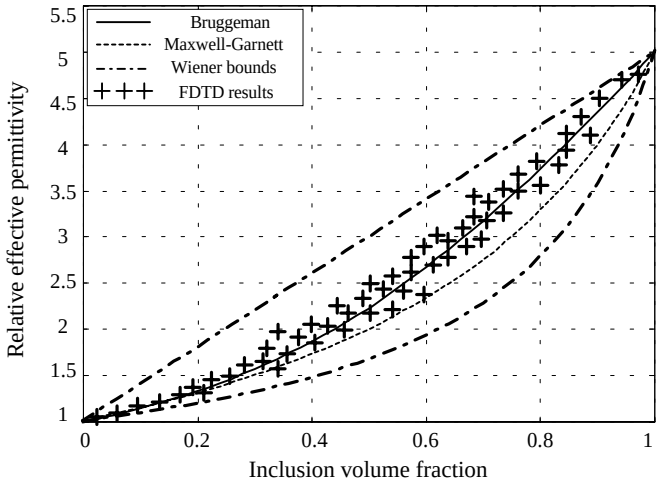

Fig.8. Effective permittivity of a mixture with $\varepsilon_i = 5$ and $\varepsilon_h = 1$ The inclusions are randomly distributed.

In Fig.7 one can see the results for a mixture with ε_i =20 and ε_h = 3.5. As the permittivity contrast grows, Bruggeman model predicts higher values of ε_{eff} than the numerical results for high volume fraction of inclusions (f > 0.5). Maxwell-Garnett rule can be used only for low volume fractions. This is natural, because the model is derived analysing a single inclusion not interacting with others, which is reasonable for low volume fractions.

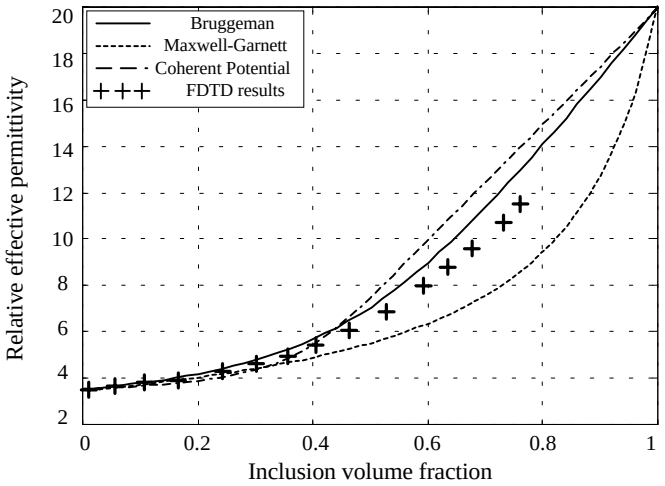

Fig.7. Effective permittivity of a mixture with $\varepsilon_i = 20$ and ε_h= 3.5 compared with theoretical models.

In Fig.8 a set of 50 simulation results for a mixture with randomly positioned inclusions are compared with Maxwell-Garnett and Bruggeman models. In every simulation both the volume fraction and positioning of inclusions were randomly chosen. Therefore, each sample has a permittivity that may differ from the value of another sample having an identical volume fraction because of their different structure. For low volume fractions results converge to a single value because the probability of inclusion overlapping and forming complex structures is low. This means that different samples do not differ in the type of their microstructure. The same happens in the case of high volume fractions when most of the inclusions overlap every time the simulation is carried out. Overlapping of inclusions allows volume fractions up to one to be achieved.

All the results in Fig.8 lie between the Wiener bounds. Numerical results are in very good agreement with the Bruggeman formula. The Maxwell-Garnett formula is applicable for low volume fractions and low contrast between the permittivities of the two phases.

VI. Conclusion

This paper presented a numerical approach based on the common Finite Difference Time Domain method for obtaining the effective permittivity value for two-phase lossless mixtures with periodical and random arrangements of inclusions. The numerical results were compared to the predictions of some well-known theoretical models. Best agreement was obtained with the Bruggeman rule.

The reported numeric technique can be easily extended to multiphase mixtures and various shapes of inclusions.

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