Effective Permittivity at the Interface of Dispersive Dielectrics in FDTD

Dijana Popovic, *Student Member, IEEE*, and Michal Okoniewski, *Senior Member, IEEE*

***Abstract*—A simple treatment of E-field component tangential to dispersive media interfaces in FDTD is introduced. The method uses concepts from the auxiliary differential equations method to average the constitutive parameters. The cases of a wave propagating in a coaxial line and of an open-ended coaxial line radiating into the dispersive media are investigated. Results show that the simulations could be significantly erroneous if the interface is not handled properly.**

***Index Terms*—Auxiliary differential equations method, dispersive materials, FDTD, material interfaces.**

I. Introduction

RECURSIVE convolution (RC) methods [1] and auxiliary differential equation (ADE) method [2] are effective ways of handling dispersive dielectrics in the finite-difference time-domain (FDTD) method. However, to the best of our knowledge, a correct method of assigning effective dielectric parameters at the interface of two dispersive media has not been proposed yet and is still an active research area even for simple, nondispersive media [3], [4].

Currently, dispersive dielectrics in the FDTD simulation space are aligned with the mesh, and the permittivity at the interface simply assigned to one of the two media. This effectively displaces the interface by half a cell, as depicted in Fig. 1 for a cylindrical FDTD formulation. Thus, errors in the reflection coefficient phase are induced due to the spatial displacement, and in magnitude due to the discontinuity at the E-field components normal to the interface.

The extent of these errors is problem specific. In the case of a geometrically homogeneous waveguide filled with two dispersive dielectrics, displacing the boundary by half a cell should only induce errors in the phase of the reflection coefficient, while the errors in the magnitude should be minimal. On the other hand, the errors can be relatively large for more complex structures, such as an open-ended coaxial line radiating into a dielectric half space. Due to complex field behavior at the aperture, the induced errors in both magnitude and phase are substantial and not easy to correct. Assigning the dielectric parameters of one of the dielectrics to the tangential E-field components has an effect similar to retracting or extending the dielectric in this line by half a cell, which can have a large effect on the calculated reflection coefficient [5].

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The authors are with the Electrical and Computer Engineering Department at the University of Calgary, Calgary, AB, T2N 1N4, Canada (e-mail: michal@enel.ucalgary.ca).

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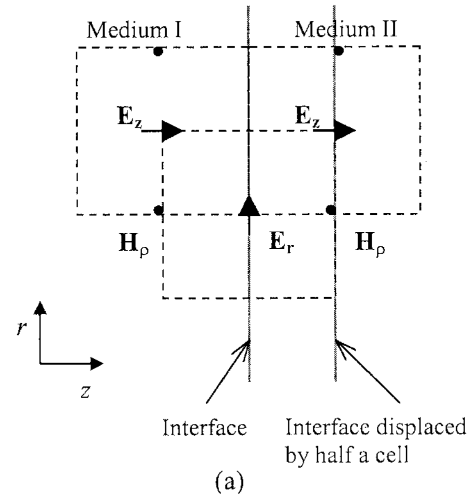

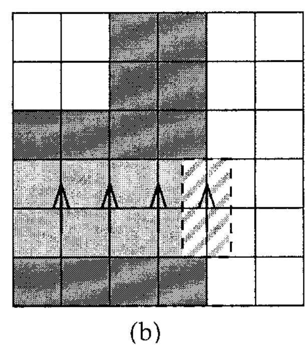

Fig. 1. (a) Dielectric boundary alignment in the 2-D cylindrical FDTD grid and (b) geometry of the open-ended coaxial line radiating into dielectric half-space. The arrows show E_r components.

II. Formulation

The proposed method is suitable for both Debye and Lorentz media, however for the sake of simplicity, the attention in this letter is given to Debye media only.

Following the ADE formulation introduced in [2], the Ampere's law equation in the time domain is expressed as

$$\nabla \times \mathbf{H}(t) = \varepsilon_0 \varepsilon_\infty \frac{\partial}{\partial t}\mathbf{E}(t) + \sigma \mathbf{E}(t) + \sum_k^P \mathbf{J}_k(t) \qquad (1)$$

where ε_0 is the permittivity of free space, ε_∞ is the dispersive dielectric permittivity at optical frequencies, σ is the material conductivity, and $\mathbf{J}_k$ are the polarization currents for each pole k.

Debye media polarization current is defined as [2]

$$\frac{d}{dt}\mathbf{J}_k = \varepsilon_0 (\varepsilon_s - \varepsilon_\infty) \frac{A_k}{\tau_k}\mathbf{E} - \frac{1}{\tau_k}\mathbf{J}_k \qquad (2)$$

where ε_s is the static permittivity, A_k is the amplitude and τ_k is the relaxation time of each pole k.

In a case where the dielectric boundary runs through the FDTD cell in parallel to the FDTD mesh, the effective permittivity for the tangential E-field component, as is the case for nondispersive materials, is the weighted arithmetic mean of the permittivities in the cell. Thus, using (1) and continuity of electric field

$$\varepsilon_{\infty,eff} = \varepsilon_0 \frac{1}{A} \int\int_A \varepsilon_\infty \cdot dA \tag{3}$$

$$\sigma_{eff} = \frac{1}{A} \int\int_A \sigma \cdot dA \tag{4}$$

where A represents the area of an FDTD cell corresponding to the electric field tangential to the interface, while ε and σ are functions of the position. In the simplest case of the interface aligned with the FDTD mesh, (3)–(4) are simple averages of the properties of two media, e.g., $\varepsilon_{\infty,eff} = 0.5\left(\varepsilon_\infty^I + \varepsilon_\infty^{II}\right)$.

In a similar manner, the polarization currents need to be averaged across the cell:

$$J_T = \frac{1}{A}\left\{\int\int_{A^I} \sum_k^{P^I} \mathbf{J}_k^I(t) \cdot dA + \int\int_{A^{II}} \sum_k^{P^{II}} \mathbf{J}_k^{II}(t) \cdot dA\right\} \tag{5}$$

where super indices I and II correspond to media I and II, respectively. It is useful to consider (5) for the simplest and most practical case where the media interface is aligned with the FDTD mesh. Under such conditions, (5) is simply

$$J_T = \frac{1}{2}\sum_k^{P^I} \mathbf{J}_k^I(t) + \frac{1}{2}\sum_k^{P^{II}} \mathbf{J}_k^{II}(t). \tag{6}$$

This equation can be interpreted as describing a new effective medium at the interface, with the number of poles equal to the sum of the poles of each of the medium I and II, and each pole having half the original amplitude. For a more complex case, involving multiple media, the effective material assigned to the tangential field component has the number of poles equal to the total number of poles for all dielectrics in the cell and amplitude of each pole is weighted proportionally to the occupied area. Note that the relaxation times for all poles remain unchanged.

III. Experiment

Two test cases are considered. The first has been designed to demonstrate a structure that is not particularly sensitive to the treatment of media interfaces. In this test a wave propagating in a coaxial waveguide filled with teflon (nondispersive) and water (dispersive) is considered. In the second test, designed to illustrate a structure for which inappropriate treatment of the interface leads to large errors, an open-ended, teflon coaxial line radiating into a water half-space is analyzed. In both cases a 2-D body-of-revolution [6] cylindrical FDTD code is used.

For each experiment, three averaging methods were investigated and compared: 1) proposed averaging scheme, and assignment of dielectric parameters to either 2) water or 3) teflon at the interface. A uniform, dense grid of 0.1 mm was used in all cases. The results were then compared to the theoretical calculations for the reflection in a coaxial line, and to the FDTD simulations of teflon retracted or bulging past the end of the open-ended coaxial line by 50 μm (the proposed averaging technique was used in these simulations).

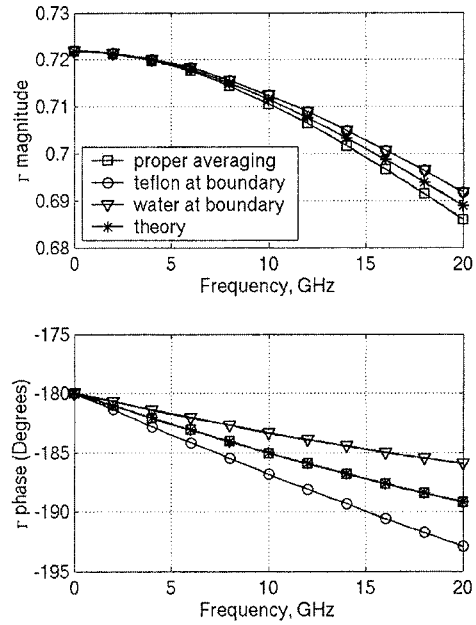

Fig. 2. Propagation of waves in a geometrically homogeneous coaxial line partially filled with water for three different dielectric parameter assignments to the tangential E_r components.

IV. Discussion

The results for the coaxial line are shown in Fig. 2. The reflection coefficient calculated using proper averaging at the interface and the theoretical reflection coefficient calculated in Matlab agree completely in phase and within 0.4% in the magnitude. When the boundary is displaced by improper parameter assignment, the expected change in the phase is

$$\Delta\Phi = 2\left(\frac{2\pi f\sqrt{\varepsilon_r}}{c}\right) l \tag{7}$$

where f is the frequency of propagation, c is the speed of light, and l is the displacement in meters. At 20 GHz this amounts to 3.48°, and is indeed the phase difference seen in Fig. 2 between the proper averaging curve and the ones showing water or teflon boundary. The reflection coefficient magnitude error for the same case has increased to 1%. These errors likely result from the improper treatment of normal electric field (E_z), which has a discontinuity at the shifted boundary.

The errors are much more pronounced in the case of the open-ended coaxial line radiating into dispersive media (Fig. 3). When the dielectric parameters assigned at the interface are equal to one of the media, a 12% (teflon) and 8% (water) error in the reflection coefficient magnitude is observed at 20 GHz. The errors in phase seem to be more significant at lower

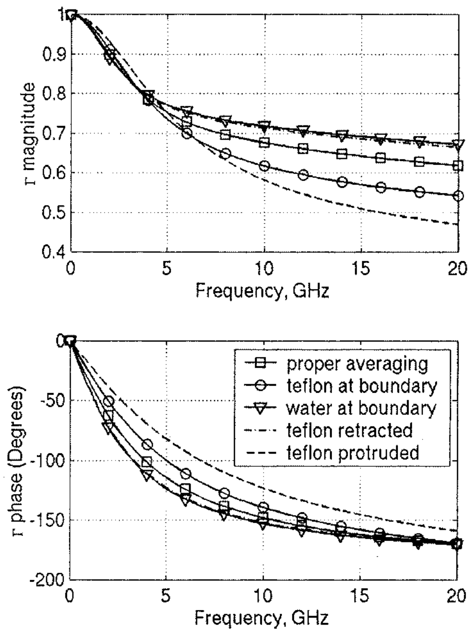

Fig. 3. Radiation of an open-ended teflon coaxial line into the water half-space for three different dielectric parameter assignments to the tangential E_r components.

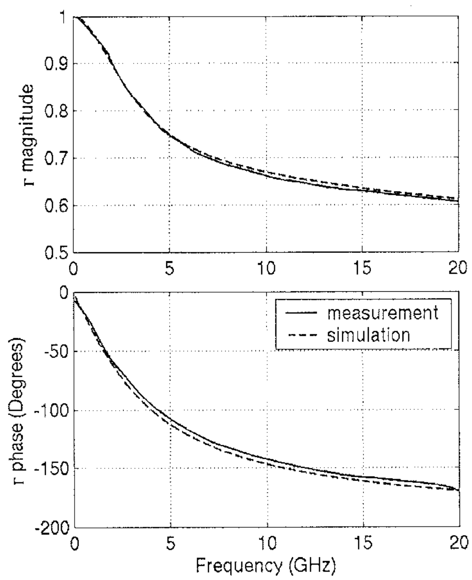

Fig. 4. Comparison of measured and simulated reflection coefficient for teflon-filled open-ended coaxial line radiating into water. The grid spacing in the z-direction is 50 μm.

frequencies and can be as high as 15°, while the differences at 20 GHz are about 1°.

It is interesting to compare the results of improper averaging of dielectric with accurate computations of open-end probe with teflon retracting or protruding 50 μm past the end of the probe. Assigning water parameters to the interface when $dz = 100\,\mu m$ gives similar results as simulations of teflon retracting into the probe by 50 μm (with magnitude difference of 1% as expected since the interface is inside the coax line). On the other hand, assigning teflon parameters to the interface induces discontinuities for the normal and tangential E_z components around the aperture, and the agreement with the simulations of teflon protruding by 50 μm is not very good. The two curves however show similar behavior when compared to the results obtained using proper averaging at the interface.

Finally, Fig. 4 shows very good agreement between measurement and numerical results using the above averaging technique for dispersive dielectric interface.

V. Conclusion

Improper averaging of dielectric parameters at the interface of dispersive media may lead to significant errors. For boundaries parallel to FDTD mesh, the averaged dispersive parameters are weighed arithmetic mean of permittivity parameters and pole amplitudes. The number of poles in the effective medium is equal to the total number of poles of the dispersive media in the cell, while the relaxation parameters of each pole remain unchanged. The new method provides for accurate method of simulation of structures involving dispersive media interfaces.

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