State-Space Approach to the FDTD Formulation for Dispersive Media

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Abstract - A novel procedure for the FDTD formulation for dispersive media is proposed. With this procedure, a dispersive medium is modeled as a time-invariant discrete system described in terms of its state-space equations. These equations are suitable for direct incorporation into the FDTD algorithm, allowing the wave propagation in general nth-order linear dispersive media to be analyzed by the FDTD method.

I. INTRODUCTION

In recent years a considerable effort has been made to extend the finite-difference time-domain (FDTD) method to the treatment of dispersive materials. In addition to its ability to handle dispersive media, this numerical technique has the flexibility to make it a powerful tool for the efficient and accurate analysis of a number of interesting electromagnetic problems, including the study of potential health hazards of high-power EM radiation and medical applications such as hyperthermia therapy.

Two approaches have been proposed in the application of the FDTD formulation to dispersive media: one approach essentially consists in transforming the frequency-domain constitutive relations to the time domain by using the convolution theorem [1]; and the other is based on taking the inverse Fourier transform to express the constitutive relations as high-order ordinary differential equations (ODEs) in the time domain [2,3].

This paper introduces an alternative approach based on modeling a dispersive medium as a linear time-invariant discrete system. Such a medium can then be described by a system of state-space equations. While maintaining the same accuracy as the high-order ODE approach, this new formulation saves approximately half of the computer storage requirements. The accuracy of this novel formulation is illustrated by a comparison between the exact and the numerical permittivity. The validity of this approach is demonstrated by applying it to the determination of the dispersion characteristics of a rectangular waveguide filled with a Lorentz medium. The propagation and attenuation constants are obtained by adapting a recently proposed 2D-FDTD formulation for dispersion analysis to the present problem [4]. A good agreement has been obtained between the exact results and those calculated by the FDTD method.

II. FDTD TREATMENT OF DISPERSIVE MEDIA

Maxwell's time-dependent curl equations are

$$\mu_0 \frac{\partial \vec{H}}{\partial t} = -\nabla \times \vec{E}, \tag{1a}$$

$$\frac{\partial \vec{D}}{\partial t} = \nabla \times \vec{H}, \tag{1b}$$

where $\vec{E}$ and $\vec{H}$ are the electric and the magnetic field strength, respectively, $\vec{D}$ the electric displacement and μ_0 the permeability of free space. For simplicity, nonpermeable media have been assumed in (1a). In addition to (1), an electric constitutive equation that relates $\vec{E}$ to $\vec{D}$ must be considered. For linear, isotropic and dispersive media, this equation can be expressed, in the frequency domain, as

$$\vec{D}(\omega) = \epsilon(\omega)\vec{E}(\omega) = (\epsilon_\infty + \epsilon_0 \chi(\omega))\vec{E}(\omega), \tag{2}$$

where $\epsilon(\omega)$ and $\chi(\omega)$ are the permittivity and susceptibility functions, respectively, ϵ_0 is the permittivity of free space and ϵ_∞ is the infinite frequency permittivity. Usually, $\chi(\omega)$ is obtained theoretically or by measurements. In this paper, we assume the following rational form for a general order-N dispersive medium

$$\chi(\omega) = \frac{b_0 (j\omega)^M + b_1 (j\omega)^{M-1} + \cdots + b_{M-1} j\omega + b_M}{a_0 (j\omega)^N + a_1 (j\omega)^{N-1} + \cdots + a_{N-1} j\omega + a_N}, \tag{3}$$

with $N \geq M$ to guarantee causality, and where $a_0, \ldots, a_N$ and $b_0, \ldots, b_M$ are constants.

The extended FDTD method for treatment of dispersive media leads to an iterative time-domain algorithm with three steps in each time iteration: first, $\vec{H}$ is updated by using the difference form of (1a); second, the difference form of (1b) is used to obtain $\vec{D}$, and third, $\vec{E}$ is updated by using an appropriate discretized time-domain model of (2). The first and second steps are common to the nondispersive FDTD method while the third step must be introduced to take into account the dispersive nature of the media. The next section introduces a formulation to carry out the third step efficiently.

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III. STATE-SPACE APPROACH

Although this technique can be used for the FDTD treatment of nth-order dispersive media described by susceptibility functions of the form (3), for the sake of brevity, its application will be illustrated for a medium with a Lorentz-type permittivity [5]

$$\frac{\vec{D}(\omega)}{\vec{E}(\omega)} = \epsilon(\omega) = \epsilon_\infty + \frac{(\epsilon_s - \epsilon_\infty)\,\omega_1^2}{-\omega^2 + 2j\omega\,\delta_1 + \omega_1^2}, \tag{4}$$

where ϵ_s is the zero frequency permittivity, ω_1 is a resonant frequency and δ_1 a damping coefficient.

This permittivity can be viewed as the transfer function of a time-invariant linear system. There are three ways to describe such a system in the time domain: the convolution, the high-order ODE and the state-space approaches. This third procedure can be directly derived from (4). However, we prefer first to obtain a high-order ODE from (4), and then to obtain, in a second step, a state-space description of the system under consideration.

Taking into account that $\mathscr{F}\,[d/dt] = j\,\omega$, we can easily obtain the inverse Fourier transform of (4), resulting in the following second-order ODE

$$\begin{aligned}\frac{d^2\vec{D}(t)}{dt^2} + 2\delta_1\frac{d\vec{D}(t)}{dt} + \omega_1^2\vec{D}(t) &= \\ \epsilon_\infty\frac{d^2\vec{E}(t)}{dt^2} + 2\epsilon_\infty\delta_1\frac{d\vec{E}(t)}{dt} &+ \epsilon_s\,\omega_1^2\vec{E}(t).\end{aligned} \tag{5}$$

Discretizing the above equation by using central finite-differences in time, we obtain a difference equation for each field component

$$\begin{aligned}c_0 D^{n+1} + c_1 D^n + c_2 D^{n-1} &= \\ E^{n+1} + d_1 E^n &+ d_2 E^{n-1},\end{aligned} \tag{6}$$

where $c_0 = 1/\epsilon_\infty$, $c_1 = (\omega_1^2\Delta t^2 - 2)/h$, $c_2 = (1 - \delta_1\Delta t)/h$, $d_1 = (\epsilon_s\omega_1^2\Delta t^2 - 2\epsilon_\infty)/h$, $d_2 = \epsilon_\infty(1 - \delta_1\Delta t)/h$, with $h = \epsilon_\infty(1 + \delta_1\Delta t)$. In equation (6) the superscript n denotes the time $t = n\Delta t$, where Δt is the time step. According to the high-order ODE approach, once (6) has been obtained, it would be solved for E^{n+1} and directly incorporated as the third step of the FDTD algorithm. Alternatively, (6) can be interpreted as a difference equation that governs a time-domain discrete system. Consequently, the dispersive medium admits a mathematical description in terms of a system of state-space equations. The following state variables are defined [6]

$$v_0^{n-1} = E^{n-1} - \beta_0 D^{n-1}, \tag{7a}$$

$$v_1^{n-1} = v_0^n - \beta_1 D^{n-1}, \tag{7b}$$

where $\beta_0 = c_0$ and $\beta_1 = c_1 - d_1\beta_0$. Using these state variables, we obtain from (6) the following state-space equations

$$v_0^{n+1} = v_1^n + \beta_1 D^n, \tag{8a}$$

$$v_1^{n+1} = -d_2 v_0^n - d_1 v_1^n + \beta_2 D^n, \tag{8b}$$

and the output equation

$$E^{n-1} = v_0^{n-1} + \beta_0 D^{n-1}, \tag{9}$$

where in (8) $\beta_2 = c_2 - d_1\beta_1 - d_2\beta_0$.

For an efficient incorporation of these equations into the FDTD algorithm, v_0 should be eliminated and the system (8,9) rearranged in the form

$$E^{n+1} = v_1^n + \beta_1 D^n + \beta_0 D^{n+1}, \tag{10a}$$

$$v_1^{n+1} = -d_2 E^n - d_1 v_1^n + (d_2\beta_0 + \beta_2) D^n. \tag{10b}$$

These equations can now be used to carry out the third step of the FDTD method for a Lorentz medium. Note that, in comparison to the nondispersive case, the implementation of (6) in the FDTD algorithm requires three additional variables in the computer storage whereas that of (10) only requires two.

IV. NUMERICAL PERMITTIVITY

In the FDTD numerical domain the dielectric properties of a Lorentz medium are modeled by (10). To assess how accurate they are, the numerical permittivity can be derived and compared with (4). As in the derivation of the numerical dispersion equation, substitution of wave solutions of the form $\vec{F}^n = \vec{F}_0\exp(j\,\omega\,n\,\Delta t)$, in (10), or equivalently in (6), gives the numerical permittivity, ϵ^{FDTD}, as $D_0 = \epsilon^{FDTD}(\omega)\,E_0$, where

$$\epsilon^{FDTD} = \epsilon_\infty + \frac{(\epsilon_s - \epsilon_\infty)\,\omega_1^2\Delta t^2}{-4\sin^2(\theta_t) + j2\,\delta_1\sin(2\theta_t)\,\Delta t + \omega_1^2\Delta t^2}, \tag{11}$$

with $\theta_t = \omega\,\Delta t/2$. As expected, the numerical permittivity tends to the exact permittivity as θ_t tends to zero. A comparison between $\epsilon(\omega)$ and $\epsilon^{FDTD}(\omega)$ will be presented in section VI.

V. APPLICATION

To show the validity of the above formulation, we have applied it to the determination of propagation constants in waveguides containing a Lorentz medium. In general, this is a 3-D problem that can be reduced to an equivalent 2-D problem by noticing that, for a uniform guide with an arbitrary cross-section, the functional dependence of the modes in the direction of propagation is analytically known and, consequently, the fields can be expressed as

$$\begin{Bmatrix} \vec{D}(x,y,z,t) \\ \vec{E}(x,y,z,t) \end{Bmatrix} = \begin{Bmatrix} \vec{d}_t(x,y,t) \\ \vec{e}_t(x,y,t) \end{Bmatrix} \cos(\beta z) + \begin{Bmatrix} \vec{d}_z(x,y,t) \\ \vec{e}_z(x,y,t) \end{Bmatrix} \sin(\beta z), \qquad (12a)$$

$$\vec{H}(x,y,z,t) = \vec{h}_t(x,y,t)\sin(\beta z) + \vec{h}_z(x,y,t)\cos(\beta z), \qquad (12b)$$

where β is the propagation constant, z the direction of propagation and the subscript t denotes the transverse field.

Substituting the above expressions into (1) and then discretizing the resulting set of 2D-equations by using central finite-differences, we obtain the following difference equations (for simplicity only TE_{n0} modes are considered).

$$h_x^{n+1/2}(i+1/2) = \frac{-\Delta t\,\beta}{\mu_0} e_y^n(i) + h_x^{n-1/2}(i), \qquad (13a)$$

$$h_z^{n+1/2}(i+1/2) = \frac{-\Delta t}{\mu_0} \frac{e_y^n(i+1) - e_y^n(i)}{\Delta x} + h_z^{n-1/2}(i+1/2), \qquad (13b)$$

$$d_y^{n+1}(i) = d_y^n(i) + \Delta t\left(\beta\, h_x^{n+1/2}(i) - \frac{h_z^{n+1/2}(i+1/2) - h_z^{n+1/2}(i-1/2)}{\Delta x}\right), \qquad (13c)$$

where the index i denotes the spatial position $x = i\Delta x$, and Δx the spatial discretization step. Similarly, (12) can be substituted into (10) and the resulting equations, together with (13), allow the FDTD algorithm for dispersive media to be applied to the analysis of waveguides loaded with a Lorentz medium.

Calculation of the dispersion characteristics involves selecting a desired value of the phase constant, β, calculating first the time-domain response and then obtaining the frequency-domain response (i.e. the resonant frequencies and quality factors of the resonant modes of the cross-section of the waveguide) from the spectral analysis of the time-domain response. Each pair of resonant frequencies and quality factors (f_i, Q_i) corresponds to one excited propagating mode, which has the previously fixed value of β at the frequency f_i, and an attenuation constant of $\alpha_i = (\pi f_i)/(Q_i v_{gi})$, where v_{gi} is the group velocity of the mode [7]. The complete dispersion diagram is obtained by changing the value of β and repeating this process. The group velocity is calculated from the β(f) curve.

VI. DEMONSTRATION

Figure 1 shows the exact permittivity for a Lorentz medium with $\epsilon_s = 1.2\epsilon_0$, $\epsilon = \epsilon_0$ and $2\pi\delta_1 = 1$ rad/seg as a function of the normalized angular frequency, ω/ω_1. For this case, the relative error

$$e = \frac{\epsilon^{FDTD}(\omega) - \epsilon(\omega)}{\epsilon(\omega)} \times 100, \qquad (14)$$

is depicted in figure 2 for various values of θ_t. It can be seen that the error is more important around of the resonance frequency. This error decreases in the whole frequency band as θ_t decreases.

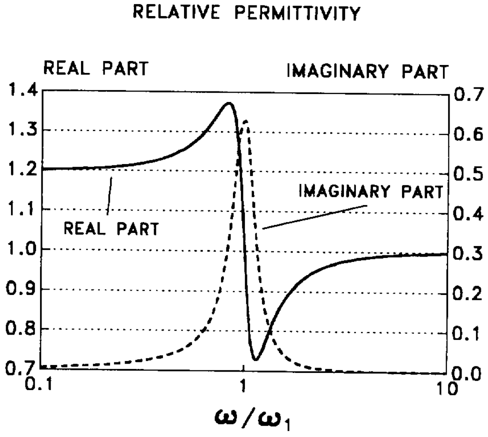

Fig. 1. Exact permittivity for a Lorentz medium with $\epsilon_s = 1.2\epsilon_0$, $\epsilon_\infty = \epsilon_0$ and $2\pi\delta_1 = 1$ seg^{-1}.

The dispersion diagram for the TE_{10} mode of a rectangular waveguide filled with a Lorentz medium is shown in figure 3. The results obtained with the new FDTD formulation for dispersive media have been compared with the exact solution, resulting in a good agreement with a discretization of only ten cells. In this case, the parameters of the medium are the same as in figure 1 but with $\omega_1 = 10\pi$ rad/seg and with $\delta_1 = 0$ seg^{-1}, that is, losses have not been considered. Figure 4 shows the same dispersion diagram with losses considered. As in the lossless case, FDTD results are compared with the exact solution. Good agreement is obtained in the whole frequency band except near the cut-off of the lossless TE_{10} mode. This is because, although losses have been included through (10), a pure imaginary propagation constant is assumed in (12) and, therefore, the method predicts almost the same $\beta(f)$ curve as in the lossless case. Thus, the 2D FDTD formulation for full-wave analysis of lossy waveguides gives good results only in the region $\beta \gg \alpha$.

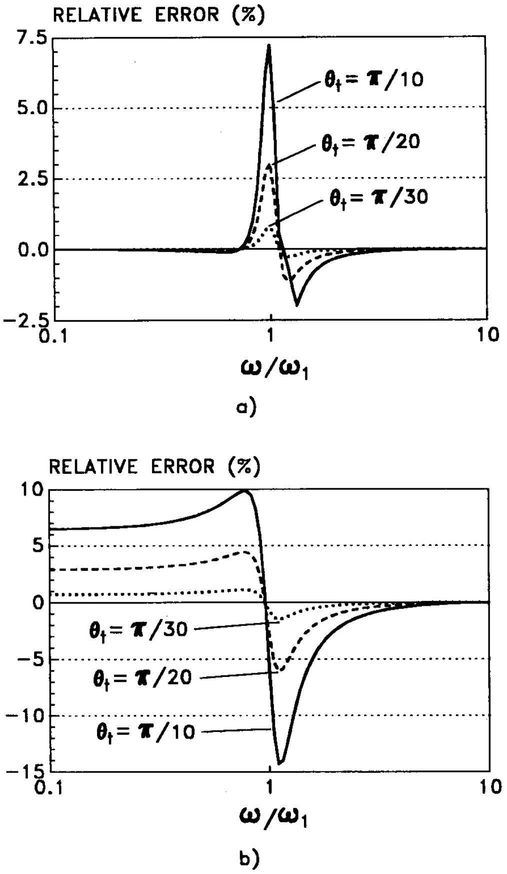

Fig. 2. Relative error between the numerical and the exact permittivity for various values of θ_t. The error is shown for the real (a) and imaginary (b) part of the permittivity. $\epsilon_s = 1.2\epsilon_0$, $\epsilon_\infty = \epsilon_0$ and $2\pi\delta_1 = 1$ seg^{-1}.

VII. CONCLUSIONS

The proposed state-space approach to the FDTD formulation for dispersive media is as accurate as the high-order ODE approach [2,3], and it is more efficient: the formulation for an nth-order dispersive medium requires, for each electric component and for each FDTD cell, n additional storage variables (the electric flux density D and n-1 state variables), while the high-order ODE approach needs 2n-1 variables [2].

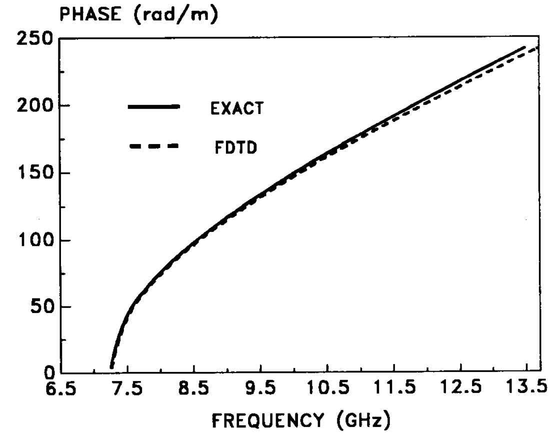

Fig. 3. Dispersion diagram for the TE_{10} mode of a WR90 waveguide filled with a Lorentz medium of $\epsilon_s = 1.2\epsilon_0$, $\epsilon_\infty = \epsilon_0$, $\omega_1 = 10\pi$ rad/seg and $\delta_1 = 0$ seg^{-1}.

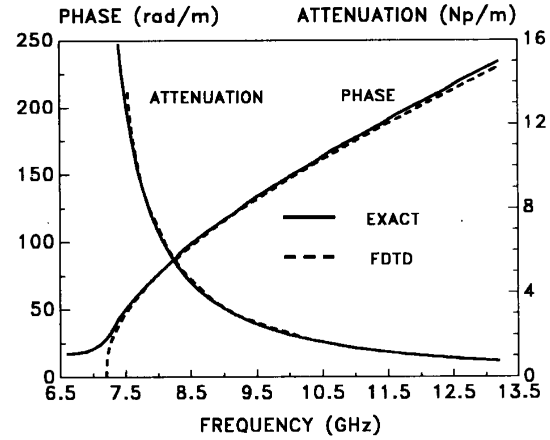

Fig. 4. Dispersion diagram for the TE_{10} mode of a WR90 waveguide filled with a Lorentz medium of $\epsilon_s = 1.2\epsilon_0$, $\epsilon_\infty = \epsilon_0$, $\omega_1 = 10\pi$ rad/seg and $\delta_1 = 5$ seg^{-1}.

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