NEW CONCEPTS FOR HARBOUR PROTECTION, LITTORAL SECURITY AND SHALLOW-WATER ACOUSTIC COMMUNICATION

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A FREQUENCY DEPENDENT FINITE DIFFERENCE TIME
DOMAIN FORMULATION FOR TIME DOMAIN RESONANCE
BEHAVIOUR OF DISPERSIVE MATERIALS

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If a dielectric is immersed in an electromagnetic field with the electric strength vector, the
medium becomes polarized. The electric field strength induces the polarization
vector can be viewed macroscopically as a volume density of dipole moments. In the
case of the polarization, medium is known as a dispersive media. This paper describes
two different ways (as a solution of recursive convolution and motion equation) to
perform finite difference time domain (FDTD) formulation of the single order dispersive
materials in order to investigate time domain resonance behaviours. For this aim, forced
time-domain oscillations in a cavity filled with a dispersive dielectric are studied. The
cavity is bounded by a singly connected and closed perfect electric conductor surface.
The numerical results for a single order dispersive material (the water is chosen as an
example) are obtained by using the solution of the recursive convolution and the motion
equation. The comparison between the results, which is obtained in two ways, shows
excellent agreement.

1 Introduction

The finite difference time domain (FDTD) method has been widely used to analyze the
electromagnetic phenomena. FDTD scheme based on the discretization of Maxwell’s
equation in space and time with cubic cells was firstly applied to Maxwell’s equations
by Yee [5]. Then FDTD solutions have been extended to include lossy dielectrics,
scattering problems, and a large geometries and applications [4].

The frequency dependent materials become more and more important in many
applications [3,4]. In this manner two ways are present for dispersive material analysis
in FDTD method. First way is to obtain the time domain transformation of the frequency
domain constitutive relations and second way is to solve the equation of motions
together with Maxwell’s equations.

First way is based on the evaluation of the convolution integral for the electric field
and susceptibility function of the material, recursively. This approach is known as
recursive convolution (RC) and it is used for materials with the Debye form of
frequency dependent permittivity [2]. Second way is based on the solution of the linearized motion equation in differential form, recursively. This approach is known as auxiliary differential equation (ADE).

One of the important examples of the single order Debye dispersive material is the water. In this paper, FDTD formulations of single order Debye dispersive materials (for water) are obtained by RC and ADE method. By using these approaches (RC and ADE), the resonance behaviours of the water in a cubic cavity having perfectly conductor walls are investigated and the results (time responses in different cavity modes) are compared.

2 FDTD Modeling of Dispersive Medium by RC and ADE methods

FDTD is one of the well-known methods for numerical solution of electromagnetic problems in the time domain. [4]. In the conventional FDTD, Maxwell's equations

\[ \nabla \times \mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t} \]  

\[ \nabla \times \mathbf{H} = \frac{\partial \mathbf{D}}{\partial t} \]  

are discretized in the terms of \( \mathbf{E} \) and \( \mathbf{H} \) to obtain field update equation. Where \( \mathbf{E} = \mathbf{E} \hat{\mathbf{e}}_i \) is electric field vector (V/m), \( \mathbf{H} = \mathbf{H} \hat{\mathbf{e}}_i \) is magnetic field vector (A/m), \( \mathbf{B} = \mathbf{B} \hat{\mathbf{e}}_i \) is magnetic induction vector (T), \( \mathbf{D} = \mathbf{D} \hat{\mathbf{e}}_i \) is displacement vector (C/m²) and \( \hat{\mathbf{e}}_i \), \( i = x, y, z \) is unit vector. In the case of simple media (\( \varepsilon \) and \( \mu \) are some scalars), the constitutive relations \( \mathbf{D} = \varepsilon \mathbf{E} \) and \( \mathbf{B} = \mu \mathbf{H} \) where \( \varepsilon \) is dielectric permittivity and \( \mu \) is magnetic permeability. But in the case of dispersive medium, the dielectric permittivity is a function of frequency \( \mathbf{D}(\omega) = \varepsilon(\omega)\mathbf{E}(\omega) \) for electrically dispersive materials and magnetically dispersive materials are straightforward. In this paper we will only deal with electrically dispersive materials like water. To perform FDTD solutions of dispersive material, two ways are present as follows.

2.1 FDTD Update Equations for Recursive Convolution (RC) Method

As above-mentioned, the dispersive medium means that \( \mathbf{D}(\omega) = \varepsilon(\omega)\mathbf{E}(\omega) \). If one takes inverse Fourier transform of \( \mathbf{D}(\omega) = \varepsilon(\omega)\mathbf{E}(\omega) \), the convolution integral will appear as

\[ \mathbf{D}(t) = \varepsilon_\infty \varepsilon_0 \mathbf{E}(t) + \varepsilon_0 \int_0^t \mathbf{E}(t - \Lambda) \chi(\Lambda) d\Lambda \]  

(3)
where $\varepsilon_0$ is the free space permittivity, $\varepsilon_\infty$ is the infinite frequency permittivity and $\chi(\Lambda)$ is the time domain susceptibility function. For single order dispersive medium, the complex permittivity of the material $\varepsilon(\omega)$

$$\varepsilon(\omega) = \varepsilon' - j\varepsilon'' = \varepsilon_\infty + \frac{\varepsilon_s - \varepsilon_\infty}{1 + j\omega\tau_0} = \varepsilon_\infty + \chi(\omega)$$

(4)

where $\tau_0$ is the relaxation time, and $\chi(\omega)$ is the frequency domain susceptibility [3]. If one takes the inverse Fourier transform of $\chi(\omega)$, $\chi(\Lambda)$ can be obtained as

$$\chi(\Lambda) = \left(\frac{\varepsilon_s - \varepsilon_\infty}{\tau_0}\right) e^{-\frac{\Lambda}{\tau_0}} \mathcal{U}(\Lambda)$$

(5)

where $\mathcal{U}(\Lambda)$ is the Heaviside function shows that the solution will be causal. To perform FDTD upgrade for RC method, it is necessary to take into account equations (1), (2), (3), (5). To simplify FDTD dispersive formulations (for explanations only), let's consider one-dimensional problem. In this case, the $x$ components of the Maxwell's curl equations can be expressed as

$$\frac{\partial H_x}{\partial t} = \frac{1}{\mu} \left[ \frac{\partial E_y}{\partial z} - \frac{\partial E_z}{\partial y} \right]$$

(6)

$$\frac{\partial D_x}{\partial t} = \frac{\partial H_z}{\partial y} - \frac{\partial H_y}{\partial z}.$$  

(7)

The other 4 equations can be obtained by cyclic rotation of the $(x, y, z)$ coordinate triplet. As we are interested in non-magnetic materials, the equation (1) can be discretized as in the conventional FDTD method [4]. Here, only the equation (7) will be discretized respecting to the FDTD method, but the derivation method of the other two is the same. The discretized form (the central differentiation) of the equation (7) is

$$D_x^{i+1/2,j,k} - D_x^{i+1/2,j,k} = H_z^{i+1/2,j+1/2,k} - H_z^{i+1/2,j-1/2,k}$$

$$\frac{\Delta y}{\Delta t}$$

$$H_y^{i+1/2,j+1/2,k} - H_y^{i+1/2,j,k-1/2}$$

$$\Delta z$$

(8)

If the left hand side of the equation (8) is calculated by using equation (3) as
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\[ D(t) \approx D(n\Delta t) = D^n = \varepsilon_{\infty}\varepsilon_0 E^n + \varepsilon_0 \int_0^{n\Delta t} E(n\Delta t - \Lambda) \chi(\Lambda) d\Lambda \]  

By using the approximation that all field values are constant over each time interval \( \Delta t \), we can rewrite the equation (9) at \( n\Delta t \).

\[ D^n = \varepsilon_{\infty}\varepsilon_0 E^n + \varepsilon_0 \sum_{m=0}^{n-1} \left\{ E^{n-m} \int_{m\Delta t}^{(m+1)\Delta t} \chi(\Lambda) d\Lambda \right\} \]  

We can also find the \( D \) value at \((n+1)\Delta t\) as

\[ D^{n+1} = \varepsilon_{\infty}\varepsilon_0 E^{n+1} + \varepsilon_0 \sum_{m=0}^{n} \left\{ E^{n+1-m} \int_{m\Delta t}^{(m+1)\Delta t} \chi(\Lambda) d\Lambda \right\}. \]

Now, using equation (10) and equation (11), \( D \) can be eliminated from the Maxwell equations after obtaining the discretized form (8). Substitution of (10) and (11) in (8) yields

\[
\begin{align*}
&\left( \varepsilon_\varepsilon_0 E_x|^{n+1}_{l+1/2,j,k} + \varepsilon_0 \sum_{m=0}^{n} \left\{ E_x|^{n+1-m}_{l+1/2,j,k} \int_{m\Delta t}^{(m+1)\Delta t} \chi(\Lambda) d\Lambda \right\} \right) \\
&- \left( \varepsilon_\varepsilon_0 E_x|^{n}_{l+1/2,j,k} + \varepsilon_0 \sum_{m=0}^{n-1} \left\{ E_x|^{n-m}_{l+1/2,j,k} \int_{m\Delta t}^{(m+1)\Delta t} \chi(\Lambda) d\Lambda \right\} \right) \\
&= \Delta t \frac{H_z|^{n+1/2}_{l+1/2,j+1/2,k} - H_z|^{n+1/2}_{l+1/2,j-1/2,k}}{\Delta y} \\
&- \Delta t \frac{H_y|^{n+1/2}_{l+1/2,j,k+1/2} - H_y|^{n+1/2}_{l+1/2,j,k-1/2}}{\Delta z}
\end{align*}
\]

In equation (12), all fields are assumed to be zero for \( t \leq 0 \). If \( \chi(t) \) is assumed to be zero, equation (6) yields \( D(t) = \varepsilon_{\infty}\varepsilon_0 E(t) \), where \( \varepsilon_{\infty} \) is equivalent to \( \varepsilon_\varepsilon \). Now the equation (12) must be rearranged for \( E_x|^{n+1}_{l+1/2,j,k} \) as
\[
E_{x|i+1/2,j,k}^{n+1} = \left( \frac{\varepsilon_0}{\varepsilon_\infty + \chi^0} \right) E_{x|i+1/2,j,k}^n + \frac{1}{\varepsilon_\infty + \chi^0} \sum_{m=0}^{n-1} E_{x|i+1/2,j,k}^{n-m} \Delta \chi^m
\]
\[
+ \frac{1}{\varepsilon_\infty + \chi^0} \frac{\Delta t}{\varepsilon_0 \Delta z} \left( H_{z|i+1/2,j+1/2,k}^{n+1/2} - H_{z|i+1/2,j-1/2,k}^{n+1/2} \right)
\]
\[
- \frac{1}{\varepsilon_\infty + \chi^0} \frac{\Delta t}{\varepsilon_0 \Delta z} \left( H_{y|i+1/2,j,k+1/2}^{n+1/2} - H_{y|i+1/2,j,k-1/2}^{n+1/2} \right)
\]

where
\[
\Delta \chi^m = \chi^m - \chi^{m+1}; \quad \chi^m = \int_{m \Delta t}^{(m+1) \Delta t} \chi(\Lambda) d\Lambda.
\]

2.2 FDTD Update Equations for Auxiliary Differential Equation (ADE) Method

In the case of dispersive materials the displacement vector can also be written as

\[
D(E) = \varepsilon_0 E + P(E) = \varepsilon_0 (E + P(E))
\]

where \( P = P(E) \) is the polarization vector, which \( P(E) \) requires solving Newton’s equation of motion [3]. \( P = P(E) \) can be viewed macroscopically as a volume density of dipole moments of the atoms per unit of time. In general, the motion equation for \( P(E) \) is nonlinear. But if the vector \( E(r,t) \) is small enough in magnitude and the dielectric is homogenous and time-invariant macroscopically, the motion equation can be linearized. Substituting \( P = \varepsilon_0 P \) for simplicity

\[
\frac{d}{dt} P + \frac{1}{\tau_0} P = \frac{\chi_s}{\tau_0} E(r,t),
\]

where parameter \( \tau_0 \) is named as the relaxation time and \( \chi_s \) is the static dielectric susceptibility and the medium is said to be dispersive because of involving time derivatives of the constitutive operator \( P(E) \),[3]. This simple approximation to the linearized Newton equation known as Debye’s equation. Since the solution way is the same for all \((x, y, z)\) components, we can use scalar form of (15) for simplicity.
\[
\frac{d}{dt} P + \frac{1}{\tau_0} P = \frac{\chi_s}{\tau_0} E \tag{16}
\]

Discretized form of (16) is

\[
\frac{P^{n+1} - P^n}{\Delta t} + \frac{1}{\tau_0} P^{n+1} = \frac{\chi_s}{\tau_0} E^{n+1}. \tag{17}
\]

By using interpolation for the half values, equation (17) yields

\[
\frac{P^{n+1} - P^n}{\Delta t} + \frac{1}{\tau_0} \left( \frac{P^{n+1} + P^n}{2} \right) = \frac{\chi_s}{\tau_0} \left( \frac{E^{n+1} + E^n}{2} \right). \tag{18}
\]

Now, we must arrange the equation (18) to obtain update equation.

\[
P^{n+1} \left( \frac{1}{\Delta t} + \frac{1}{2\tau_0} \right) = P^n \left( \frac{1}{\Delta t} - \frac{1}{2\tau_0} \right) + \frac{\chi_s}{\tau_0} \frac{E^{n+1} + E^n}{2}.
\]

For simplicity, by using

\[
TP = \frac{1}{\Delta t} + \frac{1}{2\tau_0}, \quad TM = \frac{1}{\Delta t} - \frac{1}{2\tau_0},
\]

Update equation of the polarization vector is

\[
P^{n+1} = \frac{TM}{TP} P^n + \frac{1}{TP} \frac{\chi_s}{\tau_0} \frac{E^{n+1} + E^n}{2}. \tag{19}
\]

The second required update equation is the electric field update equation. For this aim, we must discretized equation (7) respecting equation (1) as below.

\[
\frac{D^{n+1} - D^n}{\Delta t} = dD
\]

\[
\frac{\varepsilon_0 \left( E^{n+1} + P^{n+1} \right) - \varepsilon_0 \left( E^n + P^n \right)}{\Delta t} = dD \tag{20}
\]

Here, \(dD\) is discretized form of right side of equation (7) and all the \((x, y, z)\) components can be solved by the same manner. By using update equation (19), equation (20) yields electric field update equation as below.
\[
\left( E^{n+1} - E^n \right) + \left( P^{n+1} - P^n \right) = \frac{\Delta t}{\varepsilon_0} dD \tag{21}
\]

\[
E^{n+1} - E^n + \left( \frac{TM}{TP} P^n + \frac{1}{TP} \frac{\chi_s}{\tau_0} \frac{E^{n+1} + E^n}{2} \right)
- \frac{TM}{TP} P^{n-1} - \frac{1}{TP} \frac{\chi_s}{\tau_0} \frac{E^n + E^{n-1}}{2} = \frac{\Delta t}{\varepsilon_0} dD \tag{22}
\]

\[
E^{n+1} - E^n + \frac{TM}{TP} \left( P^n - P^{n-1} \right) + \frac{1}{TP} \frac{\chi_s}{2\tau_0} \left( E^{n+1} - E^{n-1} \right) = \frac{\Delta t}{\varepsilon_0} dD \tag{23}
\]

\[
E^{n+1} \left( 1 + \frac{1}{TP} \frac{\chi_s}{2\tau_0} \right) - E^n + \frac{TM}{TP} \left( P^n - P^{n-1} \right) - \frac{1}{TP} \frac{\chi_s}{2\tau_0} E^{n-1} = \frac{\Delta t}{\varepsilon_0} dD \tag{24}
\]

\[
E^{n+1} \left( 1 + \frac{1}{TP} \frac{\chi_s}{2\tau_0} \right) = E^n + \frac{1}{TP} \frac{\chi_s}{2\tau_0} E^{n-1} - \frac{TM}{TP} \left( P^n - P^{n-1} \right) + \frac{\Delta t}{\varepsilon_0} dD \tag{25}
\]

\[
E^{n+1} = \frac{1}{1 + \frac{1}{TP} \frac{\chi_s}{2\tau_0}} \left[ E^n + \frac{1}{TP} \frac{\chi_s}{2\tau_0} E^{n-1} - \frac{TM}{TP} \left( P^n - P^{n-1} \right) + \frac{\Delta t}{\varepsilon_0} dD \right] \tag{26}
\]

Now we have two update equations, first is polarization vector update equation (19) and second is electric field update equation (26). The update algorithm of the FDTD for dispersive materials can be seen below.

![Flowchart](image)

Figure 1. The dispersive update algorithm of the FDTD for ADE method.
3 Numerical results

In this investigation, the cubic cavity having perfectly electric conducting walls is filled with a dispersive material (water). A dipole source, which is infinitesimally thin and has infinite conductivity, is considered. The soft dipole source is placed in certain coordinates concerning to the desired mode simply in discretized cavity space which is filled with dispersive material, with parameters $\sigma=0$, $\varepsilon_r=81$, $\varepsilon_{er}=1$ and $\tau_0=9.4\times10^{12}$. This parameters correspond to the water. After observation time is applied long enough to reach the steady state, resonant mode is seen graphically and the results of RC and ADE methods are compared by numerical FDTD method as shown in Figure 2. It is seen in the FDTD solution that the desired cavity mode is excited for both methods with an excellent agreement.

![Figure 2. The time response of the electric field in the center of the cavity for RC and ADE methods (TM_{110}). The cavity is filled with a single order dispersive material (water).](image)

Figure 2 shows the time response of $z$ component of electric field at the center of the cavity when the source with a length $z_s=a/2$, $x_s=b/2$ in the cavity. This result is obtained by running a FDTD simulation for a cavity, filled with dispersive material (water), with dimensions ($5.10^{-3} \times 5.10^{-3} \times 5.10^{-3}$) meters that is divided into 14 unit cells in each direction and the source signal is applied for $t=3.5965\times10^{-12}$ sec. The resonance frequency of dispersive filled cavity $f=0.418115257\times10^{13}$ is calculated by the method of evolutionary approach to electromagnetic (EAE) for TM_{110} cavity mode [1]. Clearly the desired mode is excited for both methods with a good agreement.
Figure 3. (a) The electric field distribution along x-y axes at fixed $z_0=a/2$ for TM$_{220}$ mode. The source is placed at $x_0=a/4$, $y_0=b/4$ in the cavity.  
(b) RC-ADE comparison for TM$_{220}$ cavity mode.
Figure 3a shows the field distribution of the z component of electric field for cubic cavity along x-y axes at fixed z=a/2 coordinate when the source is placed in the base coordinates x_r=a/4, y_r=b/4 in the cavity. Color bar indicates the amplitude of the electric field and axis coordinates act as cell numbers. Operational frequency is f=0.8450355167x10^{13} Hz for TM_{220} cavity mode. The resonance frequency of the filled cavity is again calculated analytically by EAE [1]. Given results are obtained at t=0.92103x10^{-12} sec. that is enough to provide stability of electromagnetic oscillation. Figure 3b shows the comparison of the electric field time responses obtained by two methods for TM_{220} cavity mode. Clearly the desired mode is excited for both methods with a good agreement.

4 Discussion

The FDTD formulation of the first order depressive material is obtained by using recursive convolution (RC) and auxiliary differential equation (ADE) method in order to analyze the resonance behaviours of the water. The numerical results show that the excellent agreement is present for RC and ADE methods. It is understood from the results that in the case of water, the resonance frequency is shifted according to empty cavity resonance frequency. It is worth noting that frequency shift occurs because of not conductivity (lossy) of water. It occurs due to dispersive nature of the water means that electrical dipoles are present in the case of electromagnetic wave incidence. Moreover it is seen that field distribution of filled cavity with water is similar to the empty cavity field distribution.

This knowledge is especially important for different applications including microwave heating systems and the dielectric permittivity research in the case of broadband applications.

As a future work it is aimed to investigate second order dispersive materials (more realistic model of the dispersive material) in the different shaped cavities with non-monochromatic sources (impulse, pulse, Walsh function type and so on).

References