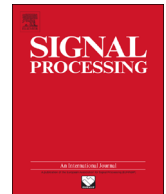




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A novel FDTD formulation based on fractional derivatives for dispersive Havriliak–Negami media

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ABSTRACT

A novel finite-difference time-domain (FDTD) scheme modeling the electromagnetic pulse propagation in Havriliak–Negami dispersive media is proposed. In traditional FDTD methods, the main drawback occurring in the evaluation of the electromagnetic propagation is the approximation of the fractional derivatives appearing in the Havriliak–Negami model equation. In order to overcome this problem, we have developed a novel FDTD scheme based on the direct solution of the time-domain Maxwell equations by using the Riemann–Liouville operator for fractional differentiation. The scheme can be easily applied to other dispersive material models such as Debye, Cole–Cole and Cole–Davidson. Different examples relevant to plane wave propagation in a variety of dispersive media are analyzed. The numerical results obtained by means of the proposed FDTD scheme are found to be in good accordance with those obtained implementing analytical method based on Fourier transformation over a wide frequency range. Moreover, the feasibility of the proposed method is demonstrated by simulating the transient wave propagation in slabs of dispersive materials.

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1. Introduction

Recently, researches on the interaction between electromagnetic waves and biological tissues have received increasing attention due to their promising applications in the area of bioelectromagnetics. In fact, the application of electric field pulses has opened a new gateway to tumor treatment since their capability to induce significant morphological and functional changes in biological cells and tissues [1–6] as well as in molecular biology by promoting the understanding of molecular mechanisms of cells.

Despite substantial progress in experimental measurements in dielectric spectroscopy, the modern state of the theory of dielectric relaxation remains unsatisfactory. The lack of data and accurate models, in wide frequency ranges, for complex dielectric properties of biological tissues has been an obstacle for both theoretical and experimental studies of their interaction with the electromagnetic field. In fact, the various biological tissues in the human body are characterized by anomalies of the dynamic dielectric properties resulting in a strong dispersion of dielectric susceptibility. This dispersion, can be explained by considering that the disordered nature and microstructure of the systems, the common property of fractal physiological structures and that power-law long-term memory effects yield a wide spectrum of relaxation

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times [7]. As a result, the time-domain response is generally non-symmetric and markedly different from that of the simple Debye dielectrics.

It is well known that an accurate representation of the experimental dielectric response in frequency domain of complex biological tissues usually cannot be described by a simple exponential expression with a single relaxation time. At present, a number of empirical relationships including Cole–Cole (CC), Cole–Davidson (CD) and Havriliak–Negami (HN) expressions have been proposed in order to fit such types of dielectric spectra [8–13]. In particular, HN expression provides an extended model flexibility enabling a better parametrization of the dispersive media properties and a better description of the generalized broadened asymmetric relaxation loss peak.

FDTD algorithm has been proven to be one of the most powerful computational methods in electromagnetics to model the wave propagation in various complex media [14–16], such as biological materials. In particular, taking into account that the frequency-domain representation of the HN complex permittivity exhibits fractional powers of angular frequency $j\omega$, the conventional FDTD algorithm needs to be modified for implementing the approximation of fractional-order derivatives. Three major FDTD approaches have been proposed to simulate the time dependent propagation of electromagnetic waves in biological tissues: recursive convolution [17], auxiliary differential equation [18–22], and Z-transform [23–25]. In the recursive convolution approach, the convolution integral is discretized into convolution summation which is then evaluated recursively. In auxiliary differential equation method the relative complex permittivity is approximated in the frequency domain by means of rational or polynomial functions leading to a number of ordinary differential equations. In the Z-transform approach, the time-domain convolution integral is reduced to a multiplication using the Z-transform. Alternative methods based on additional differential equation involving a fractional derivative have been proposed, too [17,26]. However, the authors are unaware of any method in which the fractional operator regarding the most general HN response is directly incorporated in the FDTD scheme. To this aim, we present FDTD formulation based on Riemann–Liouville theory of fractional differentiation where the fractional derivatives are approximated using finite differences [27–30]. Three types of dispersive media, described by CC, CD and HN expressions, are treated as special cases of our general formulation. Numerical results show that the proposed FDTD scheme leads to accurate simulations in a wideband frequency range.

2. Theoretical analysis

The Havriliak and Negami function is considered as a general expression for the universal relaxation law. As a consequence, the most general approximation for frequency dependence of the complex permittivity can be expressed by two-parameters formula

$$\epsilon_{r,HN}(\omega) = \epsilon_{r\infty} + \frac{\epsilon_{rS} - \epsilon_{r\infty}}{[1 + (j\omega\tau)^{1-\alpha}]^{1-\beta}} \quad (1)$$

where ϵ_{rS} and $\epsilon_{r\infty}$ are the static and infinite frequency dielectric constants, respectively, τ is the relaxation time, $0 \leq \alpha \leq 1$ and $0 \leq \beta \leq 1$ are parameters which control the dispersion broadening. For $\alpha=0$ and $\beta=0$ Eq. (1) describes the well-known Debye model. Moreover, for $\beta=0$ and $0 \leq \alpha \leq 1$ as well as for $\alpha=0$ and $0 \leq \beta \leq 1$ the Cole–Cole and Cole–Davidson equations are obtained, respectively.

2.1. FDTD formulation

Ampere's law in combination with the material relation in frequency domain can be written as

$$\nabla \times \mathbf{H} = j\omega\epsilon_0\epsilon_{r\infty}\mathbf{E} + \mathbf{J} = j\omega\epsilon_0 \left(\epsilon_{r\infty} + \frac{\Delta\epsilon_r}{[1 + (j\omega\tau)^{1-\alpha}]^{1-\beta}} \right) \mathbf{E} \quad (2)$$

where $\Delta\epsilon_r = \epsilon_{rS} - \epsilon_{r\infty}$, and \mathbf{J} is the polarization current

$$\mathbf{J} = \frac{j\omega\epsilon_0\Delta\epsilon_r}{[1 + (j\omega\tau)^{1-\alpha}]^{1-\beta}} \mathbf{E}. \quad (3)$$

Transforming (3) in time domain yields a fractional differential equation

$$(1 + \tau^{1-\alpha} \mathcal{D}_t^{1-\alpha})^{1-\beta} \mathbf{J} = \mathcal{D}_t^{\alpha,\beta} \mathbf{J} = \epsilon_0 \Delta\epsilon_r \frac{\partial \mathbf{E}}{\partial t} \quad (4)$$

where $\mathcal{D}_t^{1-\alpha}$ is the $(1-\alpha)$ th-order fractional differential operator and

$$\mathcal{D}_t^{\alpha,\beta} = (1 + \tau^{1-\alpha} \mathcal{D}_t^{1-\alpha})^{1-\beta}.$$

Based on the approximated binomial series, Eq. (4) can be written as

$$\mathcal{D}_t^{\alpha,\beta} \mathbf{J} \approx \sum_{n=0}^{N_{\alpha,\beta}} -\tau^{n(1-\alpha)} \binom{n+\beta-2}{n} \mathcal{D}_t^{n(1-\alpha)} \mathbf{J}. \quad (5)$$

In order to choose the suitable value for $N_{\alpha,\beta}$ ensuring the desired accuracy of the relative complex permittivity, Eq. (1) has been taken into account to write the truncated binomial series as follows:

$$\underbrace{[1 + (j\omega\tau)^{(1-\alpha)}]^{1-\beta}}_{F(j\omega)} \approx \underbrace{\sum_{n=0}^{N_{\alpha,\beta}} (-1)^n \binom{n+\beta-2}{n} (j\omega\tau)^{n(1-\alpha)}}_{F^a(j\omega)} \quad (6)$$

Fig. 1 shows the contour plot of $N_{\alpha,\beta}$ versus both α and β parameters considering as stop criterion the following error function

$$\epsilon_r = \sqrt{\sum_{\omega=0}^{\omega_{\max}} \left| \frac{F(j\omega) - F^a(j\omega)}{F(j\omega)} \right|^2} \leq 10^{-3} \quad (7)$$

By numerical simulation, a good approximation is obtained by using a number of terms lower than 6. However, the approximation accuracy can be improved by increasing the number of terms.

According to the popular Riemann–Liouville definition of fractional derivatives we derive

$$\mathcal{D}_t^{n(1-\alpha)} \mathbf{J} = \frac{d^{\nu}}{dt^{\nu}} \int_0^t \frac{(t-u)^{\nu-n(1-\alpha)-1}}{\Gamma[\nu-n(1-\alpha)]} \mathbf{J} du \quad (8)$$

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