Approximating Dispersive Materials With Parameter Distributions in the Lorentz Model

Jacqueline Alvarez, Andrew Fisher, and Nathan L. Gibson

Abstract We seek to improve the accuracy of the Lorentz model by incorporating a distribution of dielectric parameters and introducing a microscopic quantity we call the random polarization. Thus the usual polarization is the macroscopic average, or expected value, of the random polarization. The forward problem in the frequency domain demonstrates the difference between the distributed and deterministic models. Using a least squares cost formulation and χ^2 significance test, we explore the parameter identification problem for saltwater data. For analysis in the time domain, we use Polynomial Chaos and the Finite Difference Time Domain methods to discretize in one dimension. We then examine two time domain inverse problems that compare interrogation signals.

1 Introduction

Electromagnetic interrogation of dispersive materials is of current interest in industry for its potential as a non-invasive method in identifying weaknesses or compositions in materials. An example is determining a material's dispersive properties through the analysis of a single transmitted ultra-wideband (UWB) pulse. Several different methods have been suggested that expand on the common Lorentz polarization model, some employing linear combinations of poles or normally distributed poles to fit models to data [5]. In this paper, however, we explore placing beta distributions on the dielectric parameters in the model.

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First we present necessary background information including Maxwell's equations, the constitutive equations, and the Lorentz model. Next we introduce random parameters and define random polarization. Then using Fourier transforms, we explore the frequency domain through the complex permittivity and present a parameter identification problem. For analysis in the time domain, we use Polynomial Chaos and the Finite Difference Time Domain (FDTD) method to discretize in one dimension. We then examine two time domain inverse problems that compare interrogation signals.

2 Background

2.1 Maxwell's Equations

We begin by presenting Maxwell's equations that describe the behavior of electromagnetic waves in free space. D is the electric flux density, E and H are the electric and magnetic fields. The magnetic permeability of free space is given by μ_0

$$\frac{\partial D}{\partial t} + J = \nabla \times H \tag{1a}$$

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

$$\nabla \cdot D = 0 \tag{1c}$$

$$\nabla \cdot B = 0 \tag{1d}$$

Next, we incorporate the constitutive laws that adapt Maxwell's equations for propagation in materials. We let $\tilde{\varepsilon}$ represent the electric permittivity which is equal to the product of the permittivity of free space and a relative permittivity ($\tilde{\varepsilon} = \varepsilon_0 \varepsilon_\infty$). The polarization in the material is given by P, defined by

$$D = \tilde{\varepsilon} E + P. \tag{2}$$

To find the equations defining electromagnetic waves in a material, we substitute the constitutive equations into Maxwell's curl equations and reduce to one dimension:

$$\tilde{\varepsilon} \frac{\partial E_x}{\partial t} = -\frac{\partial H_y}{\partial z} - \frac{\partial P_x}{\partial t} \tag{3}$$

$$\mu_0 \frac{\partial H_y}{\partial t} = -\frac{\partial E_x}{\partial z}. \tag{4}$$

From now on, we drop the subscripts so that $E(t,z) = E_x(t,z)$, $P(t,z) = P_x(t,z)$, and $H(t,z) = H_y(t,z)$.

Prior to interrogation, there are no fields or polarizations present so our initial conditions are:

$$E(0,z) = H(0,z) = P(0,z) = 0. \tag{5}$$

Our boundary conditions include the interrogating signal, $f(t)$, at $z = 0$ and a reflective surface at $z = z_0$:

$$E(t,0) = f(t) \text{ and } E(t,z_0) = 0. \tag{6}$$

2.2 Lorentz Model

There are several models that describe polarization in materials. In this paper, we focus on the Lorentz model [4] for which the physical assumption is that we can treat electrons in the material as simple harmonic oscillators. The Lorentz model is given by

$$\ddot{P} + 2\nu\dot{P} + \omega_0^2 P = \varepsilon_0 \omega_p^2 E \tag{7}$$

where ν is the damping coefficient, ω_0 is the natural resonant frequency and ω_p is the plasma frequency.

Taking the Fourier transform of (2) [4], we get $\hat{D} = \varepsilon_0 \varepsilon(\omega)\hat{E}$ where $\varepsilon(\omega)$ is called the *complex permittivity*, and is given by

$$\varepsilon(\omega) = \varepsilon_\infty + \frac{\omega_p^2}{\omega_0^2 - \omega^2 + i2\nu\omega}. \tag{8}$$

It is useful to separate (8) into its real and imaginary parts. The real part is primarily responsible for the material effect on the frequency dependent speed of wave propagation, or dispersion, while the imaginary part is primarily responsible for loss or dissipation. As such, it is common to write the imaginary part as an effective (frequency dependent) conductivity. Thus the separation is $\varepsilon(\omega) = \varepsilon_r(\omega) - i\sigma(\omega)/\omega$:

$$\varepsilon_r = \varepsilon_\infty + \frac{\omega_p^2(\omega_0^2 - \omega^2)}{(\omega_0^2 - \omega^2)^2 + 4\nu^2\omega^2} \tag{9a}$$

$$\sigma = \frac{\omega_p^2 2\nu}{(\omega_0^2 - \omega^2)^2 + 4\nu^2\omega^2}. \tag{9b}$$

2.3 Random Polarization

In this paper, we explore the effects of altering the original Lorentz model by applying a probability distribution to the resonance frequency, or rather $\eta = \omega_0^2$ (since ω_0 always appears as ω_0^2, we choose to vary ω_0^2 for simplicity). In order to use distributions of parameters with Maxwell's equations [8], we define the random Lorentz model similar to (7), but where the resonance frequency is now a random variable and $\mathscr{P}$ is the *random polarization*:

$$\ddot{\mathscr{P}} + 2\nu\dot{\mathscr{P}} + \eta\mathscr{P} = \varepsilon_0\omega_p^2 E. \tag{10}$$

Next, we declare that the macroscopic polarization P, defined in (2), is modeled by the expected value of the random polarization, where η is a random variable defined over [a,b] with probability density function $f(\eta)$ [2]:

$$P(t,z) = \mathbb{E}[\mathscr{P}] := \int_a^b \mathscr{P}(t,z;\eta)\, f(\eta)\, d(\eta). \tag{11}$$

For example, in the case of a uniform probability distribution, $f(\eta) = \frac{1}{b-a}$.

Thus, (11) along with (10) represents a more sophisticated model for the macroscopic polarization present in a material than does the simple Lorentz model given in (7). We note that the Lorentz model is a subset of the random Lorentz model which assumes a discrete distribution of parameters consisting of a single value.

3 Frequency Domain

Now we consider the frequency domain formulation of the random Lorentz model. The complex permittivity (8) becomes

$$\varepsilon(\omega;\eta) = \varepsilon_\infty + \frac{\omega_p^2}{\eta - \omega^2 + i2\nu\omega}. \tag{12}$$

An observed, measured value for the permittivity or conductivity of a material would represent a macroscopic average of a microscale phenomenon. Thus, in order to compare this random Lorentz model for complex permittivity to data, we must compute its expected value. Because η is a random variable, we must integrate over the corresponding probability distribution to find the expected complex permittivity. In the case of a uniform distribution, it turns out that there is an analytical formula [1]. Otherwise, numerical quadrature can be used.

3.1 Frequency Domain Inverse Problem

The complex permittivity describes how a signal will propagate in a Lorentz material with given parameters. The frequency domain inverse problem involves recovering the appropriate material parameters, say q, by fitting a model to experimental data. Using a least squares cost formulation, we optimize using the MATLAB `lsqnonlin` function. We consider a fixed range of frequencies, and a uniform mesh on this range. We assume that permittivity and conductivity measurements are available corresponding to these discrete frequencies. We let the permittivity and conductivity data vectors be concatenated into a single vector V_{data}. Then, given a trial set of material parameters, q, a complex permittivity model (either the deterministic Lorentz or the random Lorentz) can be evaluated at the same discrete frequencies and will produce a vector of complex permittivity values $V_{model}(q)$ to compare to the data. The residual ($R(q)$) of this process is defined as the difference between the measured data and the model estimate. The least squares cost ($F(q)$) is defined as the norm of the residual, thus

$$R = V_{data} - V_{model} \tag{13}$$

$$F = R^T R. \tag{14}$$

If the permittivity and conductivity are on the same order of magnitude, they do not need to be scaled relative to each other. Thus our parameter estimation problem is to find q such that $F(q)$ is minimized.

We want to show that random permittivities are distinct from deterministic permittivities. For example, [9] discusses how the Lorenz-Lorentz model for permittivity is actually equivalent to the shifted Lorentz model with equivalence when the inequality $\omega_p^2 \ll 6\nu\omega_0$ is satisfied. To be sure the permittivities are distinct, we apply a deterministic fit of parameters to data which comes from a uniform distribution. For comparison, we plot the deterministic permittivity, i.e., using the expected value with no distribution. Results are shown in Figure 1 where the distribution's (relative) range is the radius divided by the midpoint ($r = \frac{b-a}{b+a}$). As expected, the deterministic permittivity model was unable to fit the random permittivity data.

We now attempt to fit parameters to actual saltwater data from [10]. The fits and results are shown in Figure 2 and Table 1. The error in the deterministic model fit is twice that of the distributional model fit.

To determine if there is statistical significance between the fits, we use the hypothesis testing presented in [3]. First we let $q = (\nu,\ \mathbb{E}[\omega_0^2],\ \omega_p, r) \in Q$ where Q is

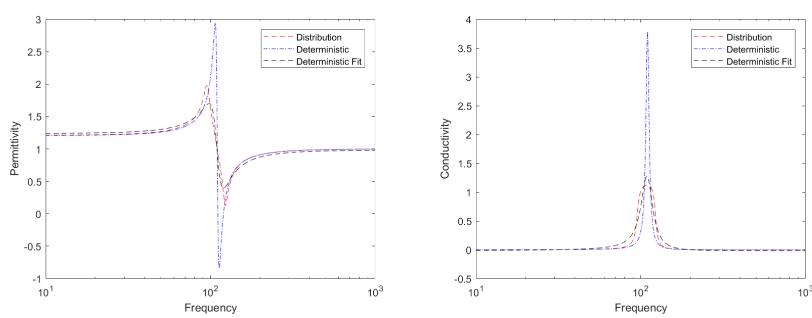

Fig. 1 Plots of the permittivity data, as well as the fitted model, for synthetic data using parameters: $\nu = 3, \omega_p = 50, \mathbb{E}[\omega_0^2] = 110$, and $r = .25$

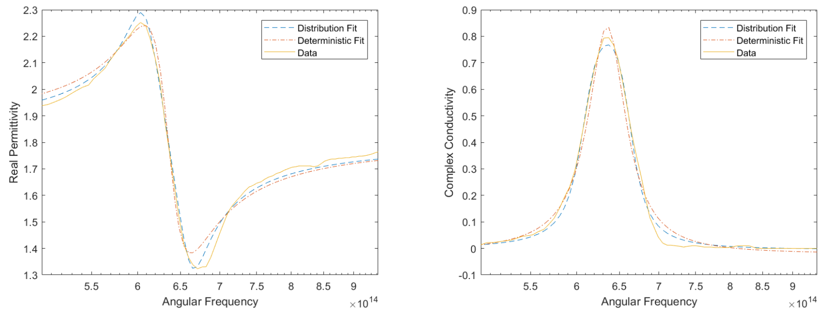

Fig. 2 Plots of the permittivity data, as well as the fitted model, for saltwater data

Table 1 Results for Saltwater Fits

Source	ε_∞	ν (1×10^{13})	ω_0 (1×10^{14})	Range	ω_p (1×10^{14})	Cost
Det. Fit	1.7931	2.7547	6.3568	–	1.7333	0.1704
Dist. Fit	1.7901	1.6112	6.3608	.0855	1.6067	0.0655

the parameter set. Then, we define Q_0 to be the set $\{Q_0 \in Q : r = 0\}$ (e.g., a discrete distribution, or a deterministic model) and let $\hat{q}_\ell$ and $\bar{q}_\ell$ denote minimizers of Q_0 and Q, respectively. We construct the hypotheses $H_0 : r = 0$ and $H_A : r \neq 0$ so that a rejection of the null hypothesis correlates to a difference in the fits. Finally, we define the test statistic:

$$U_\ell = \frac{\ell\left[F_\ell(\hat{q}_\ell) - F_\ell(\bar{q}_\ell)\right]}{F_\ell(\bar{q}_\ell)} \tag{15}$$

where ℓ is the number of data points and F_ℓ is the minimized cost.

We proceed by using a significance level α and $\chi^2(s)$ distribution with s degrees of freedom to obtain the threshold τ so that $P\left(\chi^2(s) > \tau\right) = \alpha$. We compare U_ℓ with τ, such that if $U_\ell > \tau$ we reject the null hypothesis H_0. Because the parameter r is the only degree of freedom $(s = 1)$, we refer to Table 2.

Table 2 χ^2 distribution with 1 degree of freedom

$\alpha = .25$	$\tau = 1.32$
$\alpha = .10$	$\tau = 2.71$
$\alpha = .05$	$\tau = 3.84$
$\alpha = .01$	$\tau = 6.63$
$\alpha = .001$	$\tau = 10.83$

Our simulations return $F_\ell(\hat{q}) = 0.1704$ and $F_\ell(\bar{q}) = 0.0655$ with $\ell = 79$. Plugging those values into (15) we get $U_\ell = 126.584$. Because $U_\ell >> \tau$, we reject H_0. Thus, we can conclude that a distributed model provides a statistically significantly better fit than a deterministic model.

3.2 Bimodal Data

We also consider fitting parameters to bimodal data. First, we create data using a distribution with the parameters given in Table 3. Because real data requires repeated measurements, instrument errors can be propagated. For this reason, we add normally distributed noise with $\mu = 0$ and $\sigma = .001$ to the derivatives of the bimodal data. Then we optimize with uni-modal, bi-modal, and bi-discrete model fits. Results are given in Table 3. As expected, the bi-modal model fit best matches the data with $F = 0.1118$, the uni-modal cost was 10 times larger.

Table 3 Bimodal Fit Comparison

Source	ε_∞	ν	ω_0	Range	ω_p	ν_2	$\omega_{0,2}$	Range	$\omega_{p,2}$	Cost
Data	1.000	13.000	110.000	0.200	50.000	20.000	150.000	0.300	70.000	–
Uni-modal	0.986	14.659	134.811	0.539	83.861	–	–	–	–	4.763
Bi-modal	0.978	15.079	110.918	0.179	53.817	20.573	151.327	0.262	68.229	0.1118
Bi-discrete	0.970	17.693	111.580	–	55.571	27.731	151.144	–	71.073	0.4894

4 Time Domain Discretization

Now we consider the time domain formulation of the random Lorentz model, using Polynomial Chaos to deal with the random variable ω_0^2. Polynomial Chaos is a method of solving random differential equations by expressing quantities as orthogonal polynomial expansions in the random variable [11]. We expand in the normalized Jacobi polynomials, but because they are defined on [-1,1] it is necessary to scale our distribution. Letting $\omega_0^2 = m + r\xi$ so that ξ is defined on [-1,1], we identify m and r as the center and radius of the distribution. Random polarization can now be expressed as a function of ξ,

$$\mathscr{P}(\xi,t) = \sum_{i=0}^{\infty} \alpha_i(t)\phi_i(\xi). \tag{16}$$

We refer the reader to the details in [1, 7], which include a rigorous analysis of the stability and dispersion properties of the FDTD method described here. Each of these is an extension of the methods developed in [8].

Letting $\dot{\alpha} = \beta$ we express the polynomial chaos modal equations for (10) as a system of differential equations:

$$\dot{\alpha} = \beta \tag{17a}$$

$$\dot{\beta} = -A\alpha - 2\nu I\beta + \mathbf{f}, \tag{17b}$$

where $\mathbf{f} = \hat{e}_1 \varepsilon_0 \omega_p^2 E$.

4.1 FDTD Discretization

Combining Maxwell's equations with our results from Polynomial Chaos, we have the four equations that completely determine propagation through a dielectric material. We repeat them here as a reference:

$$\varepsilon_\infty \varepsilon_0 \frac{\partial E}{\partial t} = -\frac{\partial H}{\partial z} - \beta_0 \tag{18a}$$

$$\frac{\partial H}{\partial t} = -\frac{1}{\mu_0}\frac{\partial E}{\partial z} \tag{18b}$$

$$\dot{\alpha} = \beta \tag{18c}$$

$$\dot{\beta} = -A\alpha - 2\nu I \beta + \mathbf{f}. \tag{18d}$$

It is important to note that $\frac{\partial P}{\partial t}$ is the time change in macroscopic polarization or the time change of the expected value of our random polarization. Since only the 0^{th} Jacobi polynomial is constant, we identify $\beta_0 = \frac{\partial P}{\partial t}$ with the other polynomials and coefficients determining uncertainties. This explains our substitution in (18a).

To model these equations, we discretize them according to the one-dimensional Yee Scheme [12]. The Yee Scheme implements a staggered grid where the electric field and random polarization are evaluated at integer time steps and spatial steps, while the magnetic field is evaluated at half integer time steps and spatial steps. We consider the domain $z \in [0, z_0]$ for $t \in [0, T]$, choosing integers J and N to discretize so that $\Delta z = \frac{z_0}{J}$ and $\Delta t = \frac{T}{N}$. Let $z_j = j\Delta z$ and $t^n = n\Delta t$. If U is a field variable, we define the grid function to be

$$U_j^n \approx U(x_j, t^n).$$

Our discrete initial conditions and boundary conditions are:

$$E_j^0 = \alpha_j^0 = \beta_j^0 = 0 \text{ for } 0 \le j \le J, \quad H_j^n = 0 \text{ for } 0 \le j \le J \text{ and } n \le 0,$$

$$E_0^n = f(t^n) \text{ and } E_J^n = 0 \text{ for } 0 \le n \le N.$$

First we approximate derivatives with finite differences and constant terms with averages:

$$\varepsilon_\infty \varepsilon_0 \frac{E_j^{n+1} - E_j^n}{\Delta t} = -\frac{H_{j+\frac{1}{2}}^{n+\frac{1}{2}} - H_{j-\frac{1}{2}}^{n+\frac{1}{2}}}{\Delta z} - \frac{\beta_{0,j}^{n+1} + \beta_{0,j}^n}{2} \tag{19a}$$

$$\frac{H_{j+\frac{1}{2}}^{n+\frac{1}{2}} - H_{j+\frac{1}{2}}^{n-\frac{1}{2}}}{\Delta t} = -\frac{1}{\mu_0} \frac{E_{j+1}^n - E_j^n}{\Delta z} \tag{19b}$$

$$\frac{\alpha_j^{n+1} - \alpha_j^n}{\Delta t} = \frac{\beta_j^{n+1} + \beta_j^n}{2} \tag{19c}$$

$$\frac{\beta_j^{n+1} - \beta_j^n}{\Delta t} = -A \frac{\alpha_j^{n+1} + \alpha_j^n}{2} - 2\nu I \frac{\beta_j^{n+1} + \beta_j^n}{2} + \frac{\hat{e}_1 \varepsilon_0 \omega_p^2}{2} \left[E_j^{n+1} + E_j^n \right]. \tag{19d}$$

Equations (19a), (19c), and (19d) are defined for $\{1 \leq j \leq J-1,\ 0 \leq n \leq N-1\}$ and (19b) is defined for $\{0 \leq j \leq J-1,\ 0 \leq n \leq N-1\}$.

5 Time Domain Inverse Problem

In this section, we apply our forward simulation to the time domain inverse problem. It was proven in [2] that unique solutions exist for time-domain parameter identification problems involving dispersive Maxwell's equations posed with distributions over dielectric parameters. Specifically, we wish to reconstruct the parameters of a material from noisy data collected by a receiver a distance of .252 μm into the material. We borrow parameter values from [4]. Assuming $\varepsilon_\infty = 1$ and that the interrogating signal is known, only three parameters need to optimized: ν, ω_0, and ω_p. Note that $\tau := \frac{1}{2\nu}$ and we use τ for convenience in the simulations, so the results reported below are in terms of τ.

For this time-domain parameter identification problem, the received data is observed electric field values at a discrete set of times. We collect these in a column vector V_{data}. Given a trial value of a vector of material parameters, say q, we may simulate a model of the system and collect electric field estimates at the same point in space and discrete times in order to form a vector $V_{model}(q)$. We again define the residual $R(q)$ and cost $F(q)$ as in (14) and (13). We intend to determine the dielectric parameter set q which minimizes the cost $F(q)$.

We use both Finkel's Direct global optimization program [6] and the MATLAB `lsqnonlin` function. Direct takes the n-dimensional rectangular region determined by given bounds and iteratively divides into smaller rectangles, checking for possible minimums. In this way, Direct is able to find the global minimum for functions with several local minima. On the other hand, `lsqnonlin` function uses gradient methods to converge quickly to the nearest local minimum. Our strategy is to obtain an approximate solution using Direct to optimize ω_0^2 and ω_p, and then finish optimizing all three parameters with `lsqnonlin`.

For the first inverse problem, we consider how the deterministic model fits a distribution for single frequency signals. Data is synthesized from a model using a probability distribution with a range of 0.25 and then contaminated with normally-distributed random noise with a standard deviation of ς.

We apply both deterministic and distributed fits for the 8×10^{15} frequency signal with noise of $\varsigma = 2$ for comparison. Results are given in Table 4. Even though our method accurately recovered the true values of the material, the distributed fit was unable to significantly improve on the deterministic fit.

Table 4 Fit Comparison: Freq= 8×10^{15} and $\varsigma = 2$

Source	τ (1×10^{-16})	ω_0 (1×10^{16})	Range	ω_p (1×10^{16})	Cost	Norm. Cost
Data	7	1.8	.25	2	–	–
Det. Fit	6.9489	1.7543	–	1.9697	23971	3.995
Dist. Fit	6.9819	1.8049	.2438	1.9984	23591	3.932

For the second inverse problem, we create data from the same distribution and attempt to apply deterministic and distributed fits. However, we now use a UWB as our interrogating signal:

$$f(t) = \sum_{i=1}^{n} \alpha_i \sin(f_i t) \tag{20}$$

where f_i are angular frequencies linearly spaced from 1×10^{14} to 1×10^{16} and α_i are weights determined by the beta distribution $\beta(1,3)$. Results are given in Table 5 using $n = 100$. It is clearly harder for the deterministic model to fit a UWB than a single frequency signal.

Table 5 Fit Comparison: UWB with $\varsigma = 2$

Source	τ (1×10^{-16})	ω_0 (1×10^{16})	Range	ω_p (1×10^{16})	Cost	Norm. Cost
Data	7	1.8	.25	2	–	–
Det. Fit	6.4433	1.7757	–	2.0135	25825	4.304
Dist. Fit	7.0650	1.7999	0.2493	1.9998	23441	3.907

The data supports the suggestion above that the distributed model struggles with estimating τ from the data. This is expected since a large change in τ corresponds to a small change in the cost function. Also, the distributed fit did make an appreciable difference over the cost of the deterministic fit. This agrees with our simulations in the frequency domain where the deterministic model was unable to fit parameters to the distributed permittivity over a spectrum of frequencies.

6 Conclusion

We showed in the frequency domain that applying a distribution to ω_0^2 can produce significantly better fits of parameters to real data than the deterministic Lorentz model. In the time domain, we used Polynomial Chaos and finite differences with the first order Yee Scheme to discretize the Maxwell-random Lorentz system. In [1] it was shown that the Polynomial Chaos method converged quickly for the number of polynomials used in the expansion. For the inverse problem, we compared a single frequency interrogating signal with a UWB pulse. The distributed model only fit better than the deterministic model over a range of frequencies as implied by the complex permittivity plots in the frequency domain.

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