Time domain simulation of insulating dielectric materials with non-instantaneous polarization

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Abstract: This paper presents a solution to simulate the dielectric relaxation in insulating materials using COMSOL Multiphysics in time domain. Indeed, the polarization P in a dielectric material may be divided into two parts according to the response time, the electronic polarization and the dipolar polarization. These two can respectively be regarded as a time instantaneous polarization and a time-dependent polarization, resulting from the orientation of both different types of dipoles. In the "Electric Currents" module, COMSOL Multiphysics uses an equation where the polarization is only considered as an instantaneous mechanism. However, in many cases, taking the time-dependent relaxation into account in time domain simulations is necessary. For example, dielectric relaxations modify the stress supported by an insulating material in electrical engineering or power electronics systems during transient phases. In the paper, a description of the physical mechanisms will be first presented. Then, the method proposed for their model implementation in COMSOL Multiphysics will be exposed, using the particular case of the relaxation Debye's model. The time domain parameters of the associated model will be identified from dielectric spectroscopy measurements. Examples of time domain simulation results will be given for a basic capacitor configuration under different excitation signals allowing to illustrate the proposed simulation method performance and interest.
Keywords: Electric field simulations, Dielectric relaxation, Time domain simulation, Insulation system.

Introduction

When an external electric field $\vec{E}$ is applied on a dielectric sample, a nonzero macroscopic dipole moment appears and the dielectric is polarized under the influence of the field $\vec{E}$. The mechanism of polarization deals with how a molecules or atoms are reacting to the external electric field, by forming dipoles able to be oriented. The polarization vector $\vec{P}$ is the volume density of electric dipole moments. In the linear approximation, the polarization of the dielectric sample is proportional to the strength of the electric field $\vec{E}$. If all the polarization are supposed to be instantaneous and collinear with the applied electric field, the relation between $\vec{P}$ and $\vec{E}$ is given by equation (1):

$$\vec{P}(t) = \varepsilon_0 \chi \vec{E}(t) \tag{1}$$

where ε_0 is the vacuum permittivity, and χ is the material susceptibility.

Electronic polarization, ionic polarization, dipolar polarization and interfacial polarization are some important types of polarization mechanisms[1]. When the external applied electric field applied for a sufficiently long duration is suddenly suppressed, the decay of polarization to zero is not instantaneous but takes a finite time. This is the time required for the dipoles to recover a random distribution. Similarly, following to the sudden application of a direct voltage, it takes a finite time interval before the dipole polarization will achieve its maximum value[2]. This phenomenon is described by the general term of dielectric relaxations. The relaxation time τ is used to define the time constant of a dielectric relaxation dynamics[3]. As a main reason of the energy losses in insulating materials, the study of the dielectric relaxation impact on an electrical system behavior is important.

At the start of the 20th century, Debye[3] theorized the orientational polarization phenomenon for low pressure gases. Assuming a single type of dipoles without interaction between them, if a step electric field $\overrightarrow{E_0}$ is applied at an initial time, the polarization vector $\vec{P}(t)$ will evolve in the dielectric material as represented on Figure 1, and described by the following relation :

$$\vec{P}(t) = \overrightarrow{P_\infty} + \left(\overrightarrow{P_s} - \overrightarrow{P_\infty}\right) * \left(1 - e^{-\frac{t}{\tau}}\right) \tag{2}$$

In fact, this behavior can be separated into two distinct phenomena : an instantaneous one, for which $\overrightarrow{P_\infty}$ is defined as the instantaneous polarization, followed by a non-instantaneous polarization one, with a relaxation time τ. When all the dipoles are oriented, the remaining polarization is defined as the static polarization $\overrightarrow{P_s}$.

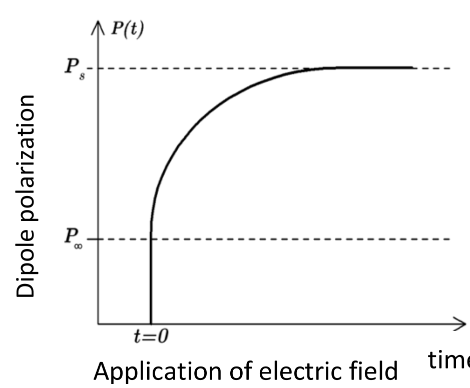


Figure 1 . Dynamic polarization for a step of electric field $\overrightarrow{E_0}$

The applied electric field $\overrightarrow{E_0}$, using equation (1) and the corresponding χ_∞ and χ_s are infinite and static susceptibilities, can be introduced into the equation (2) as follows :

$$\vec{P}(t) = \varepsilon_0 \chi_\infty \overrightarrow{E_0} + \varepsilon_0 (\chi_s - \chi_\infty) \left(1 - e^{-\frac{t}{\tau}}\right) \overrightarrow{E_0} \tag{3}$$

Based on the definitions of the electric displacement $\vec{D} = \varepsilon_0 \vec{E} + \vec{P} = \varepsilon_0 (1+\chi) \vec{E}$ and of the relative permittivity $\varepsilon = 1 + \chi$, $\vec{D}(t)$ can also be given by the equation :

$$\vec{D}(t) = \varepsilon_0 \varepsilon_\infty \overrightarrow{E_0} + \varepsilon_0 (\varepsilon_s - \varepsilon_\infty) \left(1 - e^{-\frac{t}{\tau}}\right) \overrightarrow{E_0} \tag{4}$$

with ε_∞ and ε_s corresponding to the instantaneous polarization and the long-term polarization. If ε_∞ , ε_s and τ are independent on the electric field E_0 applied, equation (4) corresponds to the step response of a first order linear system. Considering any electric field $\vec{E}(t)$ and using the Laplace transformation in time domain ($\mathrm{L}_t\{\vec{F}(t)\} = \vec{F}(s)$) the equation (4) can be generalized :

$$\vec{D}(s) = \varepsilon_0 \varepsilon_\infty \vec{E}(s) + \varepsilon_0 \frac{\varepsilon_s - \varepsilon_\infty}{1 + \tau s} \vec{E}(s) = \overrightarrow{D_\infty}(s) + \overrightarrow{D_\#}(s) \tag{5}$$

We set:

$$\overrightarrow{D_\#}(s) = \varepsilon_0 \frac{\varepsilon_s - \varepsilon_\infty}{1 + \tau s} \vec{E}(s) \tag{6}$$

The Laplace inverse transform of relations (5) and (6) leads to the following equations:

$$\vec{D}(t) = \varepsilon_0 \varepsilon_\infty \vec{E}(t) + \overrightarrow{D_\#}(t) \tag{7}$$

$$\overrightarrow{D_\#}(t) + \tau \frac{\partial \overrightarrow{D_\#}}{\partial t} = \varepsilon_0 \, (\varepsilon_s - \varepsilon_\infty) \vec{E}(t) \tag{8}$$

Hence, the system consisting in equations (7) and (8) is the one to be solved in order to take into account non instantaneous polarization in dielectric materials in time domain simulation of electrical devices for any electric field $\vec{E}$(t).

Currently, COMSOL Multiphysics only allows to take into account non instantaneous polarization mechanisms in the frequency domain by replacing s with $i\omega$ in Equation (5), can be rewritten:

$$\frac{\vec{D}(i\omega)}{\vec{E}(i\omega)} = \varepsilon_0 \varepsilon_\infty + \varepsilon_0 \frac{\varepsilon_s - \varepsilon_\infty}{1 + \tau \, i\omega} \tag{9}$$

In this case, Debye defined the complex permittivity ε^*, as a function (10) of the angular frequency as follows :

$$\varepsilon^*(i\omega) = \varepsilon_\infty + \frac{\varepsilon_s - \varepsilon_\infty}{1 + i\omega\tau} \tag{10}$$

where, ω is the angular frequency (in rad/s).

However, the frequency domain calculation only allows the users to predict the situation in the steady state of an electrical system under sinusoidal excitation (moreover requiring a linear behavior of the materials properties). Though, overvoltage or overcurrent could appear in operation transient phases of the electrical system, which cannot be predicted with the frequency domain solver. Especially, overvoltage is a critical factor in the design of electrical insulating devices for high voltage applications.

In this paper, we propose a method to be able to take into account the non-instantaneous polarization effect based on a time domain simulation, using COMSOL Multiphysics tool, in the particular case of the relaxation Debye model. Our simulations will be carried out with a basic parallel-plane capacitor, under sinus and step excitation signals.

The model and implementation in COMSOL

In general, the 'Electric Current' physics in COMSOL is used to compute the electric field, current and potential distributions of a configuration (geometry, mesh, boundaries conditions etc.). According to the conduction electric current due to the charge flow and the displacement current due to the rate of change of the electric field, the equation of the current in the dielectric medium is the generalized Ohm's law (11) where σ is the electric conductivity of the medium.

$$\vec{J}(t) = \sigma \vec{E}(t) + \frac{\partial \vec{D}(t)}{\partial t} + \vec{J_e}(t) \tag{11}$$

$$\vec{D}(t) = \varepsilon_0 \varepsilon \vec{E}(t) \tag{12}$$

But, in order to take account of the phenomenon of non-instantaneous Debye type polarization, Debye's model should be solved together with the generalized Ohm's law by replacing the equation (12) by the equations (7) and (8). The implementation of the Debye's equations in time domain ('Mathematics') will be coupled with the generalized Ohm's law (11) ('Electric current').

The relation of the electric displacement (equation (7)) must be formulated in the 'Charge conservation' boundary condition for the dielectric material with non-instantaneous polarization in the model.

The non-instantaneous electric displacement $\overrightarrow{D_\#}(t)$, is calculated coupled by the 'Partial differential equation' with the variable electric field in different directions (equation (8)).

Finally, the equations (the model) solved in COMSOL could be summary by:

$$\overrightarrow{E(t)} = -\overrightarrow{grad}\, V(t) \tag{13}$$

$$\overrightarrow{J(t)} = \sigma \overrightarrow{E(t)} + \frac{\partial \overrightarrow{D(t)}}{\partial t} + \overrightarrow{J_e(t)} \tag{14}$$

$$\vec{D}(t) = \varepsilon_0 \varepsilon_\infty \vec{E}(t) + \overrightarrow{D_\#}(t) \tag{15}$$

$$\overrightarrow{D_\#}(t) + \tau \frac{\partial \overrightarrow{D_\#}}{\partial t} = \varepsilon_0 \, (\varepsilon_s - \varepsilon_\infty) \vec{E}(t) \tag{16}$$

In the following section, examples of simulations in the time domain solving these equations will be presented. A first case will allow a comparison with the corresponding simulation in frequency domain. In order to do so, it is necessary to consider the equivalent complex permittivity, as the one obtained from spectroscopy impedance[4]. The impedance Z_{IS} (17) of a test cell made of a dielectric material metallized on both sides is defined as :

$$Z_{IS}(i\omega) = \frac{1}{C_{IS}(i\omega)i\omega} \tag{17}$$

Where the complex capacitance is given by :

$$C_{IS}(i\omega) = \varepsilon_0 \varepsilon_{IS}(i\omega)\frac{S}{e} \tag{18}$$

Where S and e are the dielectric sample surface area and thickness, and $\varepsilon_{IS}(i\omega)$ is the equivalent complex permittivity. The real $\varepsilon'(\omega)$ and imaginary $\varepsilon''(\omega)$ parts of this complex permittivity, are classically defined by the following expression :

$$\varepsilon_{IS}(i\omega) = \varepsilon'(\omega) - i\varepsilon''(\omega) \tag{19}$$

$\varepsilon'(\omega)$and $\varepsilon''(\omega)$are the required parameters to be input in COMSOL for frequency domain simulation. The relations allowing to define these two parameters in function of the Debye model parameters and the electric conductivity are :

$$\varepsilon'(\omega) = \varepsilon_\infty + \frac{(\varepsilon_s - \varepsilon_\infty)}{1 + \tau^2\omega^2} \tag{20}$$

$$\varepsilon''(\omega) = \frac{\sigma}{\omega\varepsilon_0} + \frac{\tau\omega(\varepsilon_s - \varepsilon_\infty)}{1 + \tau^2\omega^2} \tag{21}$$

Simulation examples

The performance validation of the simulation taking into account non instantaneous polarization mechanisms in the time domain, by using the proposed method, has been made considering a simple parallel plane electrode-capacitor structure. Its definition in COMSOL is presented on Figure 2, showing the 10 mm-thick dielectric material inserted between both top and bottom metallic electrodes, covered by air layers (of about 100 mm thick). The width of this structure is 500 mm. A current source is supplied to the uncharged capacitor.

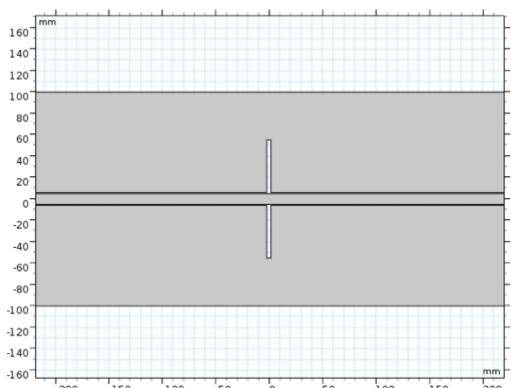


Figure 2 . The parallel-plane capacitor description in COMSOL

The dielectric material properties have been defined using σ , τ , ε_s and ε_∞ parameters, assuming a non-instantaneous polarization behavior according to the Debye's model. In all this section, the parameters σ, ε_s and ε_∞will be given the fixed values presented in Table 1, whereas the time constant τ will be specified for each simulation case. The electric field induced in the dielectric material is the simulated quantity under study. Several simulation results are presented hereafter.

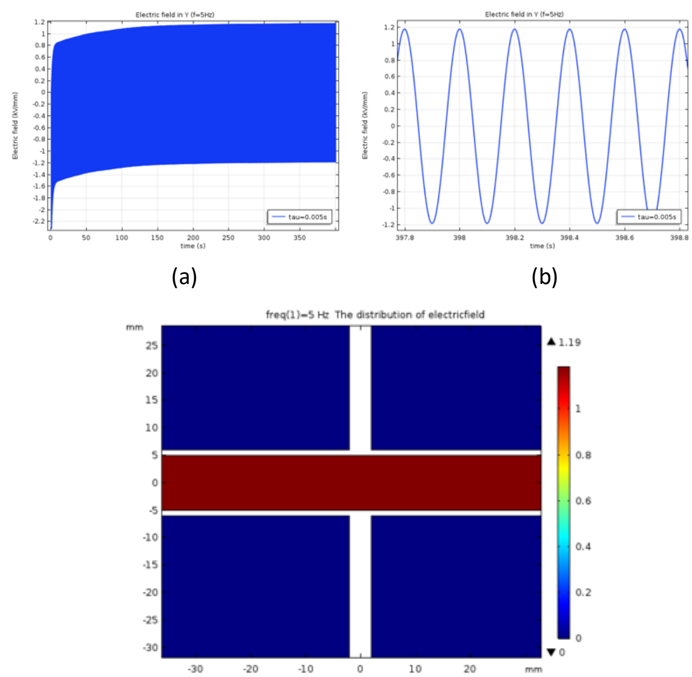
Table 1 . Simulation parameters for the relaxation dielectric medium

Property	$\sigma(S/m)$	ε_s	ε_∞
Value	$1*10^{-12}$	9	3

a. Steady state results for a sinusoidal current excitation

In order to compare the proposed method's results with COMSOL's already allowed results, a sinusoidal current excitation has been considered first, with a 0.5 mA-current magnitude (I_0) and 5 Hz-frequency (f). In this case, the non-instantaneous polarization can be taken into account by performing frequency domain calculation, deriving the real $\varepsilon'(\omega)$ and imaginary parts $\varepsilon''(\omega)$ values of the complex permittivity from equations (20) and (21).

The result obtained from the time domain simulation including our model is presented by Figure 3, which shows the electric field time dependence, from the initial transient period (after the current supply/application, supposing $I(t) = I_0$ at $t = 0s$), up to the steady state (at long enough times) of the electric field time variation.



(a) (b) (c)

Figure 3 : (a) Electric field vs Time simulated in time domain using the proposed method calculation (b) The steady state of the results in time domain (c) Simulation in frequency domain

Only the steady state electric field characteristics can be calculated in the frequency domain Figure 3(c), based on the magnitude and the phase of the complex electric field $\vec{E}(i\omega)$. By comparing both simulation results in the steady state Figure 3(b) (c), we could verify that the same electric field magnitudes, of 1.19 kV/mm, are well obtained. So this comparison attests the successful performance of our method, its validation at steady state for sinusoidal excitation, and its interest for obtaining the transient period of the simulated system.

b. Transient state results for step current excitation

The electric field of the transient phase when a step of current source is applied (of 0.5 mA), obtained from the COMSOL simulations with different constant times $\tau = 5s$, $\tau = 25s$ are shown in Figure 4. As reference data, results of the simulations which are calculated with $\varepsilon = 9$ (epsi9) and $\varepsilon = 3$ (epsi3) without Debye model are also shown (all the polarizations are then regarded as instantaneous polarizations and it means $\tau = 0s$).

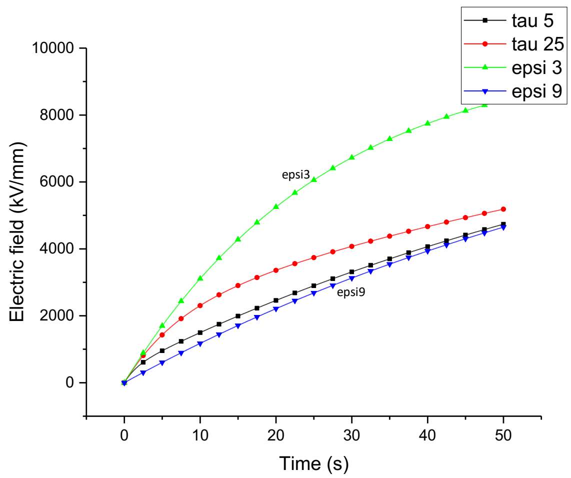


Figure 4 . Electric field (step response) vs Time in front of the electrode. Blue/green: without Debye Model $\varepsilon = 9/3$. Black/red: with Debye Model $\tau = 5/25(s)$

The results of the field with the Debye model vary between the results of 'epsi9' and 'epsi3', the Debye model describes the processes of the variety of the time dependent polarization from P_∞ to P_s. One can see the influence of the time constant τ on the velocity of the variation of the electric field in transient phase.

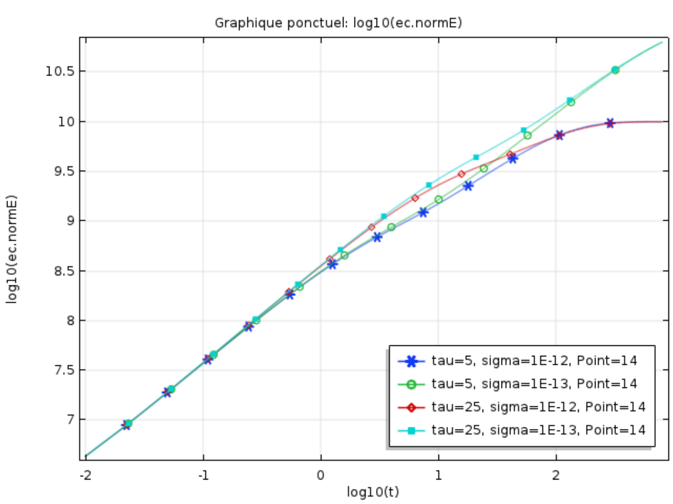
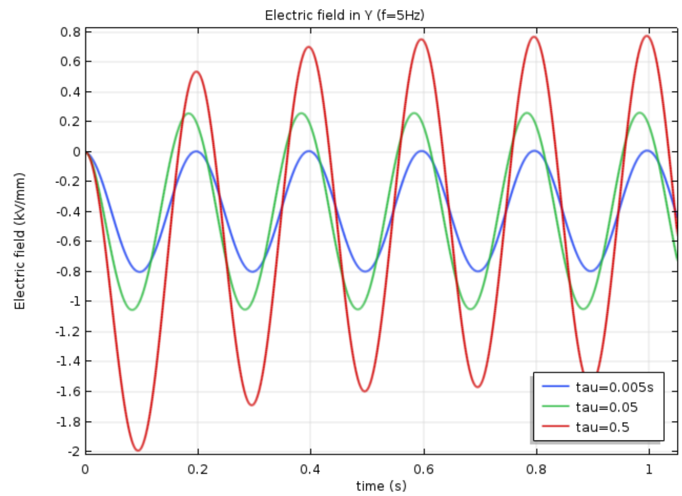


Figure 5 . Electric field (step response) vs Time in front of the electrode with different time constant in Debye model and conducivity

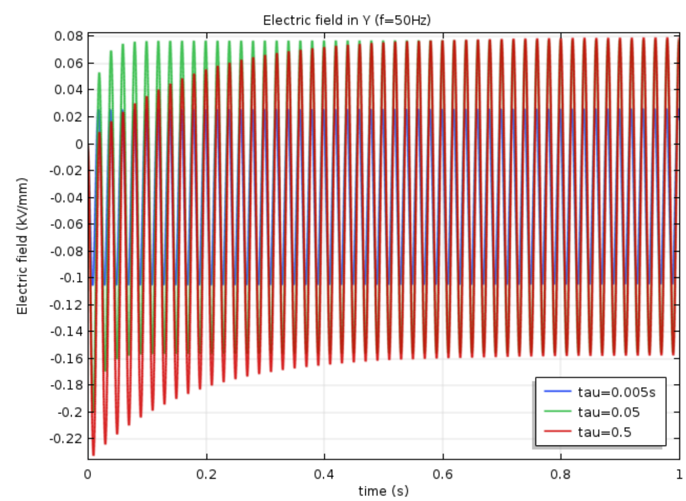
The results with different constant times ($\tau = 5s$, $\tau = 25s$) in Debye model with different conductivities ($\sigma = 10^{-13}\ S/m$, $\sigma = 10^{-12}\ S/m$) show in Figure 5. The transient period of a system without Debye model depends on both the conductivity and the permittivity of the dielectric material. The system with a smaller conductivity needs more time to achieve the steady state. The electric field varies faster with a greater τ when the step response is just applied, then it becomes slower.

c. Transient state results for sinusoidal current excitation

Figure 6 shows a sinusoidal ($f = 5Hz, 50Hz$) signal is applied on the geometry for the simulation. All material properties (σ, ε_s and ε_∞) are the same as those in previous section (Table 1).



(a)



(b)

Figure 6 . Electric field vs Time in front of the electrode with different time constants τ (a) frequency of signal $f = 5\ Hz$ (b) frequency of signal $f = 50Hz$

As the results of the sinusoidal signal show, the maximum value of the electric field (absolute peak value) in the transient period is more important than the one in the steady state. Based on the simulation results, it was observed that the transient phase is dependent on the relation between the time constant τ and the period T of the sinusoidal signal applied. As long as the time constant $\tau \ll T$, most of the non-instantaneous polarizations (including depolarizations) are completed in each period, therefore a significant difference in the amplitude could be found with different time constant. While these two parameters are in the same order of magnitude, the transient period of Debye polarization appears. For the time constant $\tau = 0.05s$, there is no significant transient overvoltage for the 5Hz-excitation in Figure 6(a). However, the transient overvoltage appears for the excitation of 50Hz in Figure 6(b).

It should also be noted that the transient phase is also influenced by the initial conditions.(not shown here)

Conclusions

The electric field is a key parameter to control for the development of higher voltage electrical insulation devices. The standard simulation method consists in solving the Poisson's equation, the generalized Ohm's law and charge conservation in the time domain with the material parameters i.e. electrical conductivity and relative permittivity, or in the frequency domain with complex permittivity. However, all polarizations are considered as instantaneous in COMSOL Multiphysics in the time domain calculation. In the frequency domain, non-instantaneous polarizations are considered but only for the steady state and the sinusoidal excitation.

In this article, we propose a solution to take into account the non-instantaneous polarization which can be applied for all types of excitation (sinus, step, square etc.). The basic geometry used allowed to prove the concept through a simple example. The steady-state results for our model when sinusoidal excitation is applied are compared with the results obtained by COMSOL in the frequency domain computation. This model can be easily integrated in more complex 3D geometries with several stacked dielectric materials and whatever the type of excitation.

The different parameters introduced by the Debye model (τ, ε_∞ , ε_s), can be easily identified from temporal measurements[6] or from more commonly by impedance spectroscopy tests.

Here, we have introduced the Debye model in the computation, because it is the most basic model to describe dielectric relaxation. Other models can be integrated such as the Cole-Cole[5], Cole-Davidson or Havriliak-Negami models, even if their implementation in time domain simulations will not be direct because of the presence of non-integer time derivatives[6].

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