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Engineering Through The Fundamentals®

COMSOL CONFERENCE 2019 BOSTON

Time Domain Analysis of Dielectric Relaxation

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Outline

- Introduction to Veryst
- Problem Background
- Generalized Debye Model
- Implementation
- Example Application – Dielectric Heating of PMMA

Introduction to Veryst

“Engineering Through the Fundamentals”

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- Multiphysics modeling
- Polymer mechanics
- PolyUMod® software
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- Microfluidics
- Materials science
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- MEMS
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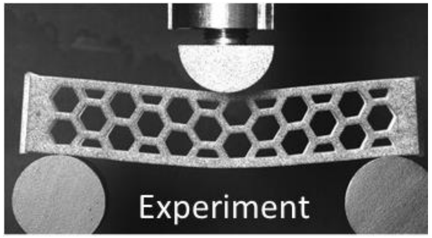
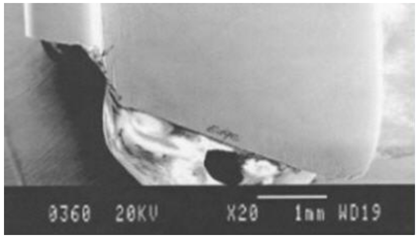
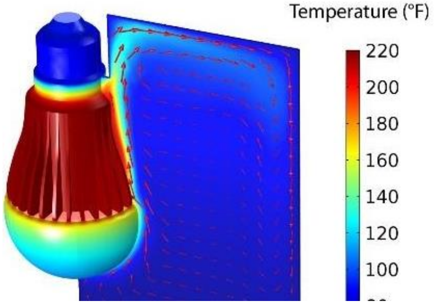
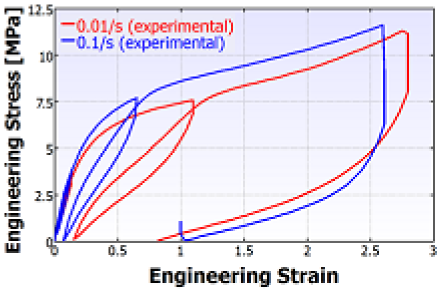
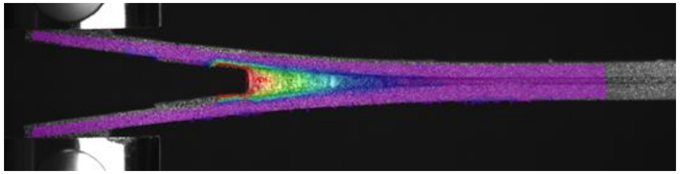
- Training classes





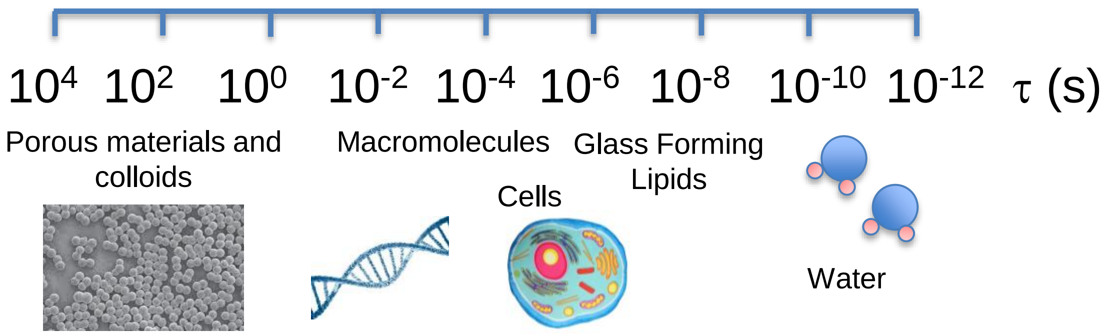






Problem Background

- Sometimes linear materials do not capture all the physics of a problem – important phenomena such as rate dependent response and losses are not captured
- Accurate descriptions of non-linear materials can be critical for developing a detailed understanding of system limitations
- In the case of a dielectric material, the polarization cannot respond instantly to an applied – field – but instead responds with a characteristic time, τ. There are also dielectric losses
- This work explores how to create realistic models of a dielectric material in the time domain



Timescale for dielectric response

Generalized Debye Model

For an isotropic material, the generalized Debye model results in the following frequency domain relationship between the electric displacement field, $\mathbf{D}$, and the electric field, $\mathbf{E}$:

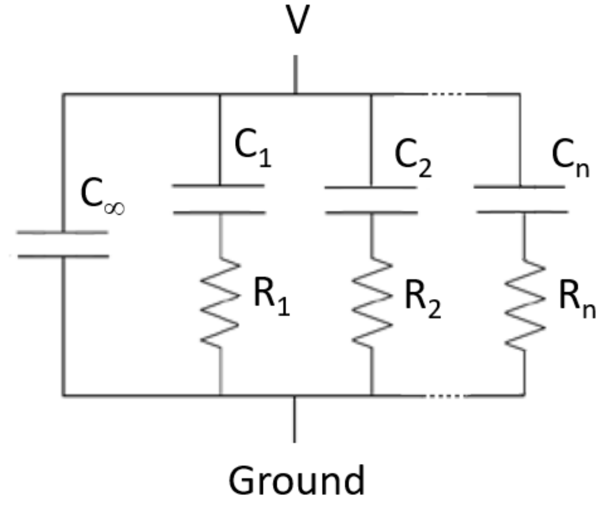
$$\mathbf{D} = \left(\varepsilon_\infty + (\varepsilon_s - \varepsilon_\infty) \sum_k \frac{g_k}{1 + i\omega\tau_k} \right) \mathbf{E}$$

where

- ε_∞ is the high frequency permittivity
- ε_s is the low frequency permittivity
- ω is the angular frequency
- τ_k is the relaxation time for the k^{th} process

and where $\sum_k g_k = 1$

Equivalent Lumped Model



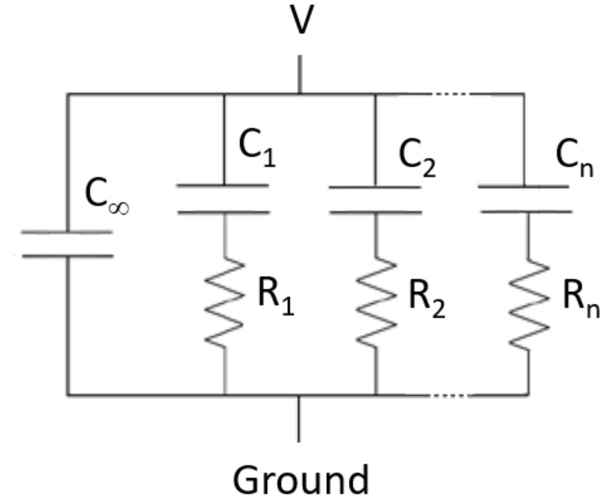
$$Q = \frac{V}{i\omega Z} = \left(C_\infty + \sum_k \frac{C_k}{1 + i\omega C_k \mathrm{R}_k} \right) V$$

Generalized Debye Model

$$\mathbf{D} = \left(\varepsilon_\infty + (\varepsilon_s - \varepsilon_\infty) \sum_k \frac{g_k}{1 + i\omega\tau_k} \right) \mathbf{E}$$

- Physically speaking, separate terms in the summation can be viewed as individual dielectric relaxation processes, associated with the polymer molecule adjusting its relaxation in different ways
- Alternatively, one can simply view the series as an empirical fit to real experimental data and arbitrarily many terms can be added to improve the fit
- The model is equivalent in form to the lumped circuit on the right

Equivalent Lumped Model

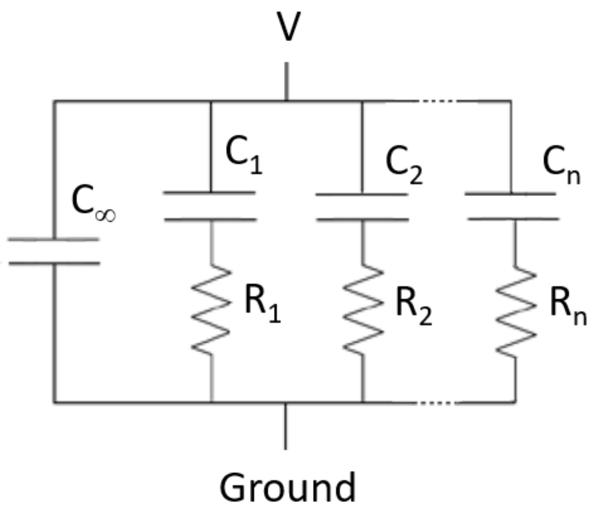


$$Q = \frac{V}{i\omega Z} = \left(C_\infty + \sum_k \frac{C_k}{1 + i\omega C_k \mathrm{R}_k} \right) V$$

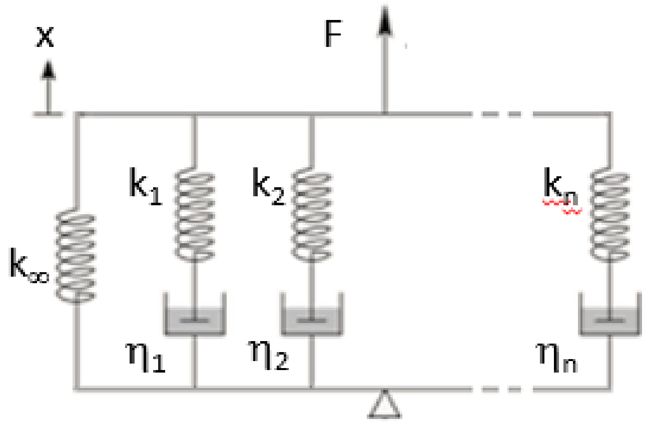
Mechanical Analog

- The electrical equivalent model has a mechanical analog – it is equivalent to the generalized Maxwell model for a viscoelastic solid
- In the electrical analog, the effect of the resistor is that the applied voltage is not entirely dropped over the capacitor – whilst in the mechanical analog a certain fraction of the displacement is taken up by the damper. Similarly the effect of the finite response time of the molecules τ_k is that the molecular polarization is initially related to only a fraction of the applied field.

Electrical Model



Equivalent Structural Mechanics Model



Time Domain Implementation

- Consider a single branch of the network in the time domain. The potential drop across the ith capacitor, V_i, can be determined from current continuity:

$$\frac{V - V_i}{R_i} = \frac{dQ_i}{dt} = C_i \frac{dV_i}{dt}$$

$$V - V_i = R_i C_i \frac{dV_i}{dt}$$

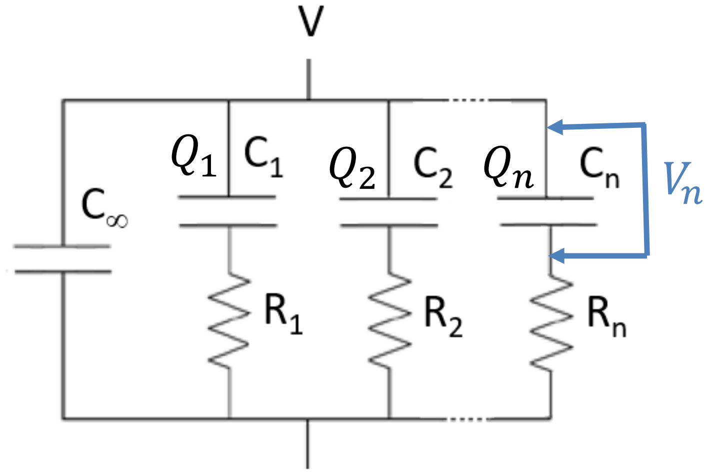
- Using the analogue, the effective field across the *ith* term in the dielectric constant is:

$$\mathbf{E} - \mathbf{E}_i = \tau_i \frac{d\mathbf{E}_i}{dt}$$

and the D-field is given by:

$$\mathbf{D} = \varepsilon_\infty \mathbf{E} + (\varepsilon_s - \varepsilon_\infty) \sum_i g_i \mathbf{E}_i$$

Equivalent Lumped Model



These terms can be written as:

$$\sum_i \boldsymbol{D}_i = \sum_i \varepsilon_i \mathbf{E}_i$$

Time Domain Implementation

- Just as the losses in the ith resistor are given by

$$P_i = I_i(V - V_i) = C_i \frac{dV_i}{dt}(V - V_i)$$

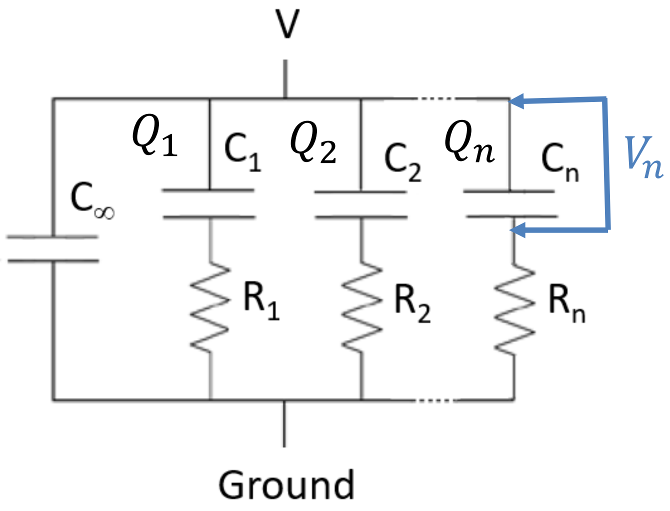
- …the losses per unit volume from the ith term in the dielectric constant are:

$$P_{v,i} = \frac{d\mathbf{D}_i}{dt} \cdot (\mathbf{E} - \mathbf{E}_i)$$

which, using the results from the previous slide, can be written in the form:

$$P_{v,i} = \tau_i \varepsilon_i \frac{d\mathbf{E}_i}{dt} \cdot \frac{d\mathbf{E}_i}{dt}$$

Equivalent Lumped Model

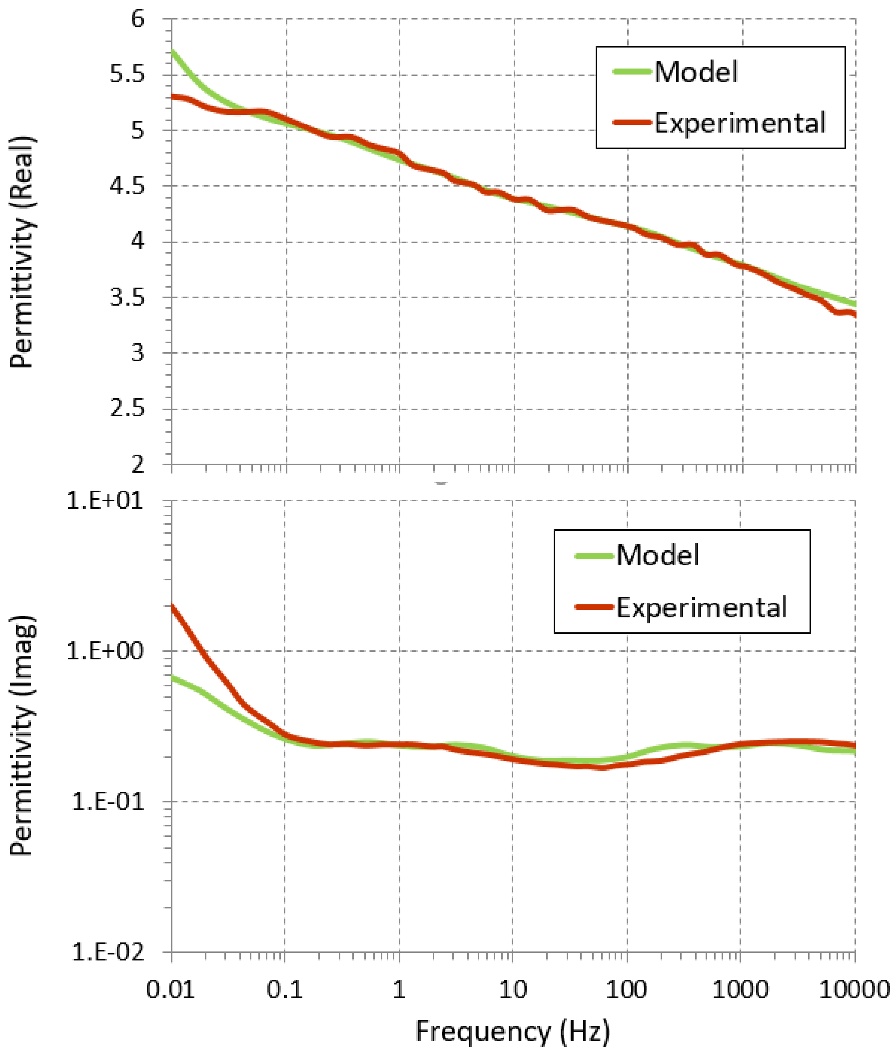


Example Material: PMMA

- Model fit to experimental data:

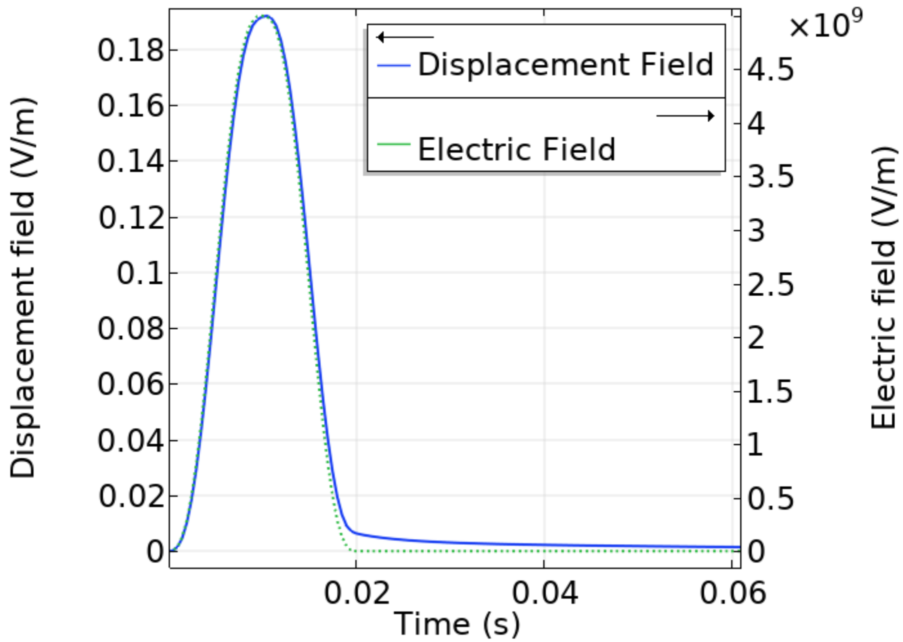
$$\mathbf{D} = \varepsilon_0 \left(\varepsilon_{\mathrm{r},0} + \sum_{i=1}^{8} \frac{\varepsilon_{r,i}}{1 + i\omega\tau_i} \right) \mathbf{E}$$

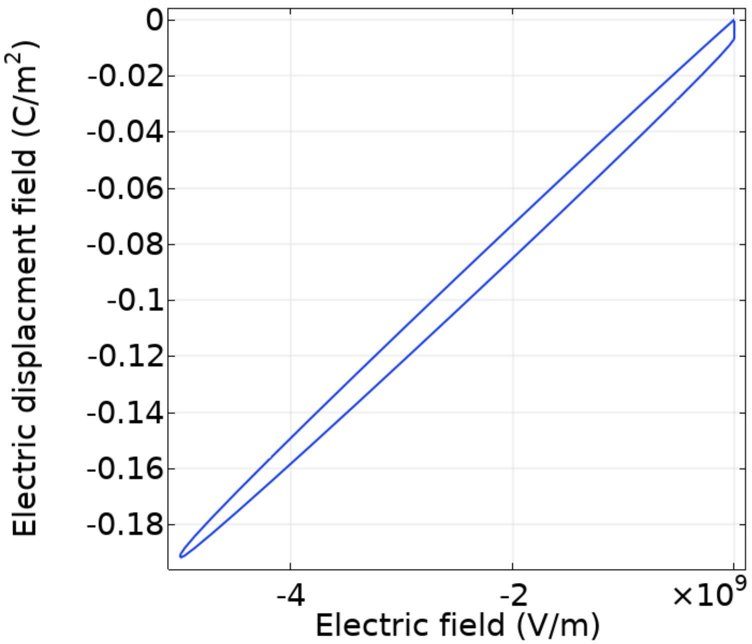
i	$\varepsilon_{r,i}$	τ (s)
0	3.19	
1	1.30	20
2	0.195	2.5
3	0.325	0.313
4	0.325	0.0391
5	0.195	4.88×10^{-3}
6	0.325	6.10×10^{-4}
7	0.325	7.63×10^{-5}
8	0.325	9.54×10^{-5}



Results for PMMA

- Phase lag between electric field and electric displacement
- Area under **E-D** curve represents heat dissipation





Note – for this demonstration example an unrealistically high electric field was applied to enhance the dielectric heating for demonstration purposes.

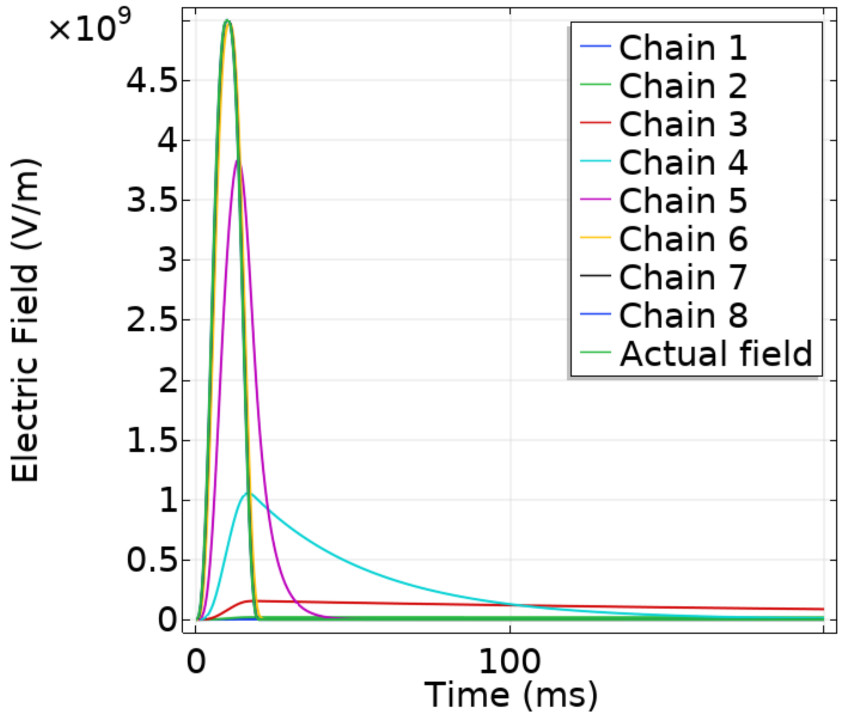
Results for PMMA

- Effective field and dissipation for each of the terms in the series

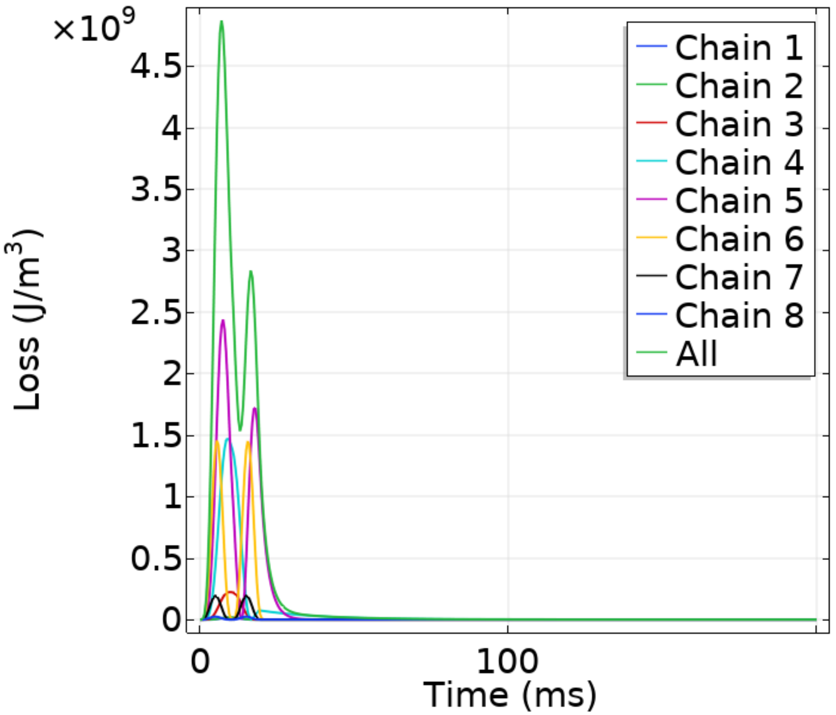
$$\boldsymbol{D} = \varepsilon_0 \left(\varepsilon_{r,0} \mathbf{E} + \sum \varepsilon_{r,i} \mathbf{E}_i \right)$$

$$P_{v,i} = \tau_i \varepsilon_i \frac{d\mathbf{E}_i}{dt} \cdot \frac{d\mathbf{E}_i}{dt}$$

Effective Electric Field for Each Term

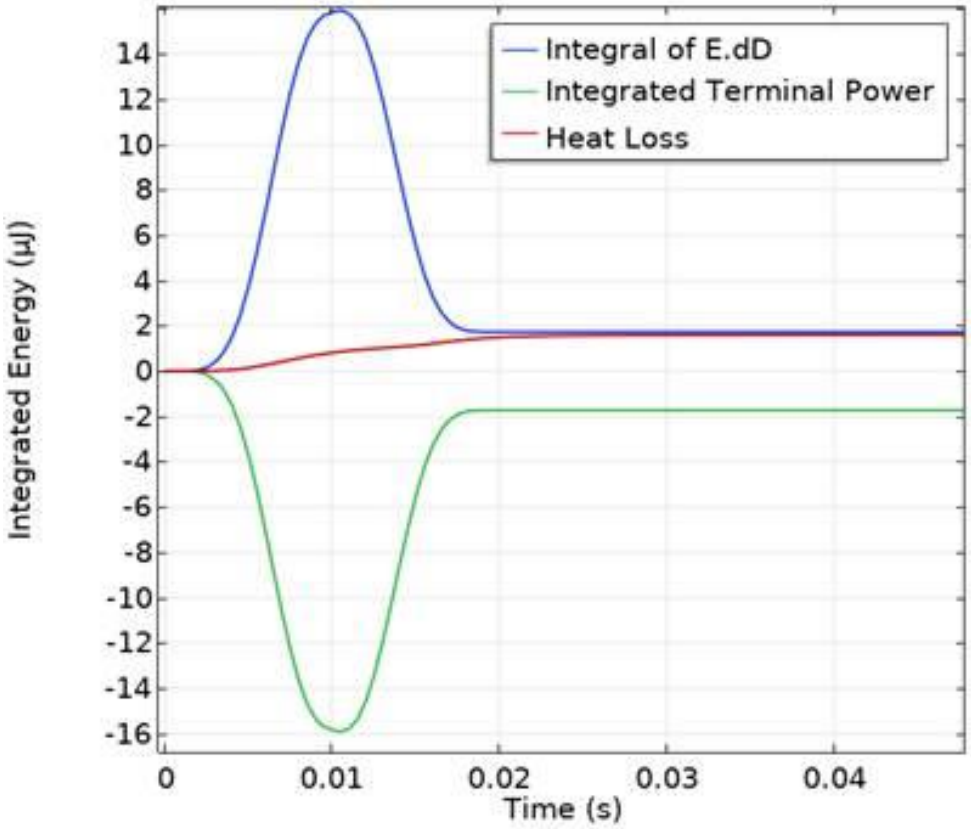


Dissipation for Each Term



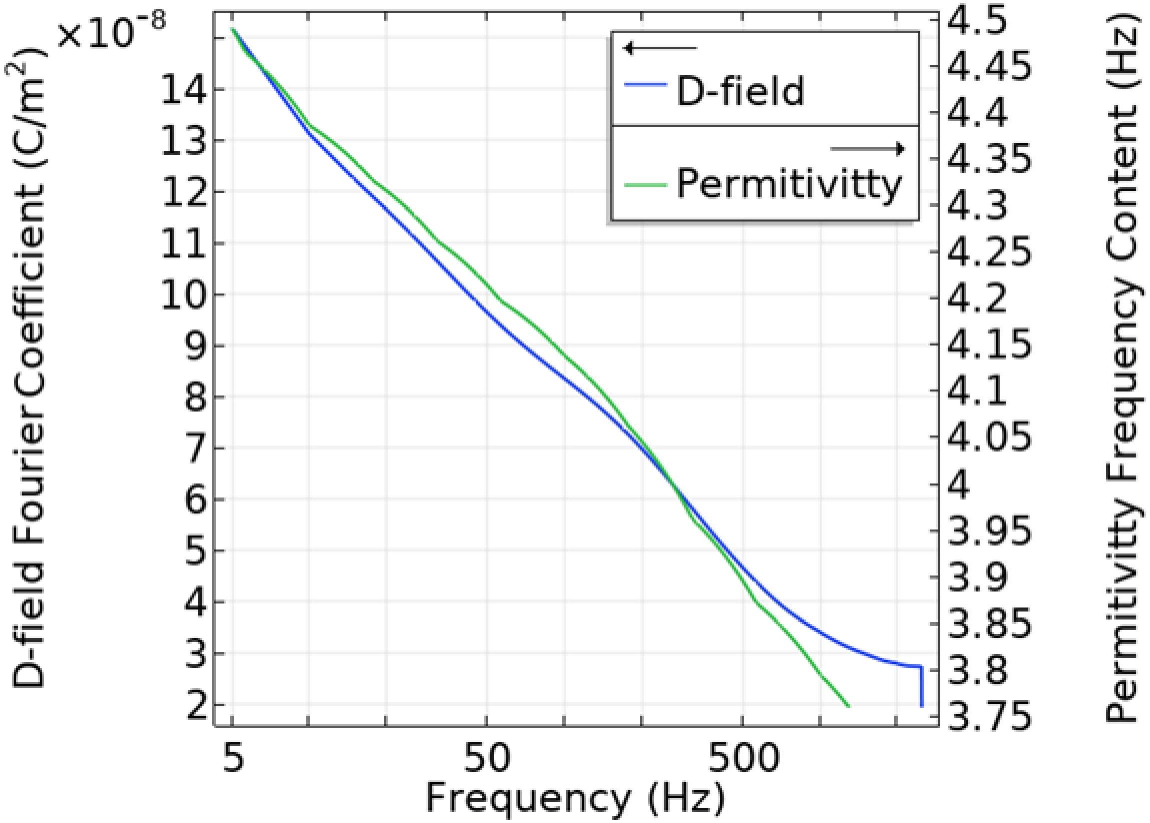
Model Validation

- Checking the energy conservation in the system results in good agreement between the power added to the system, the internal energy in the fields and the energy dissipated as heat



Model Validation

- There is reasonable agreement between the Fourier transform of the response of the dielectric to a short timescale pulse (blue curve) and the intended frequency content of the permittivity (green curve)

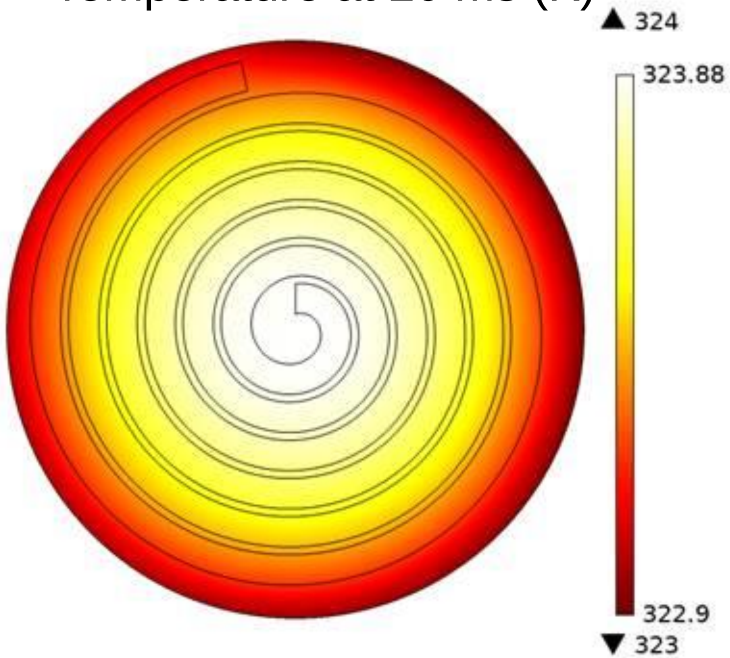


Applications

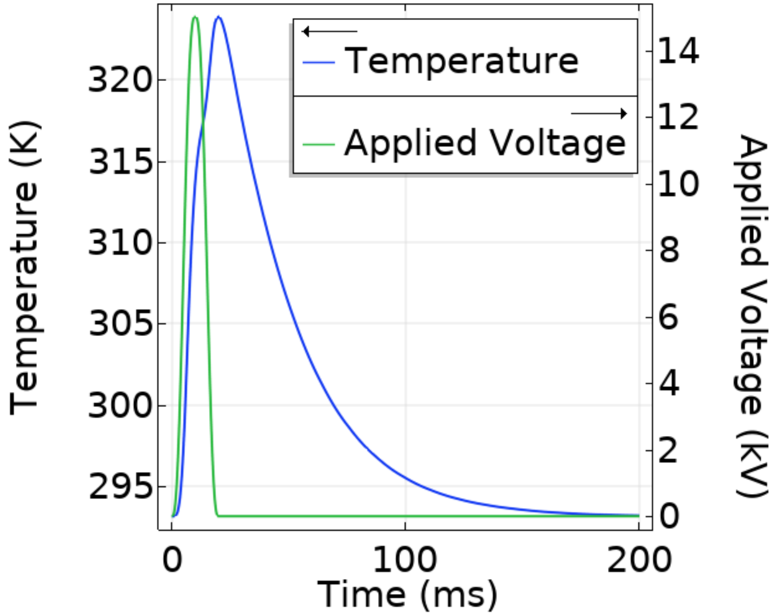
- The model can be applied to a range of different applications, including dielectric heating, impedance spectroscopy and detailed understanding of electromechanical effects in electroactive materials

Heating of an axial lead type foil capacitor

Temperature at 20 ms (K)



Temperature at Capacitor Center



Summary and Conclusions

- We have developed a time-domain technique for the finite element modeling of dielectric relaxation – based on analogies with the mechanical Prony series approach that is frequently used for modeling viscoelastic materials
- The approach employed has been validated and demonstrated to work in a simple example.
- It can be applied for the transient modeling of dielectric response in applications such as:
  - Time domain dielectric relaxation spectroscopy
  - Transient modeling of electrostatic discharge in the presence of dielectrics
  - Modeling of lightning strikes