Dielectric Modelling for a Liquid Crystal-based Optrode

Author: Hrishikesh Srinivas

Supervisor: Prof. Nigel Lovell  Co-Supervisor: Prof. François Ladouceur

Research Theme: Resources and Infrastructure for the Future

Introduction

A novel optical electrode (optrode) design based around a deformable helix liquid crystal (LC) is being investigated for sensing electrical potentials in excitable tissue (biopotentials).

Innovation and Application

Devi electrode design is based on the linear reflectance of light traversing an LC layer with an electric field applied across it. Optimisation would allow complex extracellular (e.g. neuron, cardiac tissue) biopotentials to be detected with high sensitivity by this principle (Figure 1).

Background

The dielectric constant $\varepsilon_r$ of the LC layer determines its internal polarisation $P$ in response to an external electric field $E$, and its internal displacement field $D$, all related by $D = \varepsilon_r E = \varepsilon_0 E + P$ where $\varepsilon_0$ is the permittivity of free space constant.

From measurements, $\varepsilon_r$ is not a constant material property, but has frequency dependence that has so far not been taken into account in electrical, time-dependent models of the optrode. This parameter has implications for the physics of device operation.

Approach 1: Dielectric Constant $\varepsilon_r$ in MATLAB®

The aim is to implement in a time-domain simulation the Debye dielectric response, given by

$$\varepsilon_r(\omega) = \varepsilon_\infty + \frac{\varepsilon_0 - \varepsilon_\infty}{1 + j\omega \tau}$$

with single relaxation time $\tau$, static and infinite frequency permittivities $\varepsilon_\infty, \varepsilon_0$, and $\omega = 2\pi f$.

- Multiplication in the frequency domain. $\mathbf{D}(\omega) = \varepsilon_r(\omega)\mathbf{E}(\omega)$, requires knowledge of the whole biopotential electric field $\mathbf{E}(t)$ in time.
- The time-domain equivalent is convolution, $\mathbf{D}(t) = \varepsilon_r(\omega)\mathbf{E}(\omega)\mathbf{E}(1 - \tau' t) dt'$ where the impulse response $\delta(t)'(t)$ is derived from the inverse Fourier transform of the Debye formula. This allows evaluation of $\mathbf{D}$ on each time step, but time-convolution is a non-trivial issue in COMSOL.

Is there another way?

Approach 2: Polarization $P$ in COMSOL®

We look instead at the electromagnetic relation $P = \varepsilon_r(\omega) - 1)E$:.

- Split the polarization vector $\mathbf{P}$ into induced polarization component $\mathbf{P}_i = \varepsilon_0(\omega - 1)E$, and orientational polarization component $\mathbf{P}_0 = \varepsilon_0(\omega - 1)\mathbf{E}$, so that $\mathbf{P} = \mathbf{P}_0 + \mathbf{P}_i$.
- (1) Solve for $\mathbf{P}_i$ as a dependent variable, (2) solve the differential equation $\frac{d\mathbf{P}_i}{dt} + \frac{j\omega}{\tau}\mathbf{P}_i = \varepsilon_0\mathbf{E}(t)$, and (3) add $\mathbf{P}_0$.
- Claim: specifying the above for COMSOL’s finite element method is equivalent to implementing the Debye dielectric response in the liquid crystal domain.

Verification and Implementation

Model Verification with MATLAB

The Debye response was implemented in COMSOL using the second approach and tested for a simplified 2D square geometry, with one side held at sinusoidal electric potential of $|E| = 1$ and fixed test frequency, the opposite side held at ground, and the remaining two sides insulated, bounding the liquid crystal domain.

Time-dependent solver results closely match the overall frequency response, as well as the analytical convolution formula implemented in MATLAB by the first approach.

Approach 2 was then implemented in the existing full device electrical model, with application to sensing the neuron potential generated by sinusoidal pulse stimulus current. The neuron is approximated as a branched line current source in saline solution, generating an impulse potential sampled at the top layer of the device. Copper vias conduct the biopotential electric field to the liquid crystal layer.

Summary and Further Work

- We have tested Approach 2 and shown agreement with the analytical convolution approach to the Debye model for frequency-dependent dielectric response.
- We have implemented the Debye model in a COMSOL time-domain simulation of the behaviour of the liquid crystal layer for an optrode designed to sense biopotentials.
- Next: Extend the method to simulate the Cole-Cole dielectric response, which has a better fit with measurements of the liquid crystal.

References


Acknowledgements

Many thanks to Dr. Amr AlAbed (GSLmE) and Dr. Leonardo Silvestri (EET) for their invaluable insights and expertise in tackling this modelling problem, the Optrode project team, and UNSW Faculty of Engineering for the Taste of Research opportunity.