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FINITE ELEMENT SIMULATION OF ELECTROACTIVE MECHANICAL RESPONSE OF SCLERA USING A MULTI-PHYISICS CHEMO-ELECTRO-MECHANICAL MODEL

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INTRODUCTION

Electroactive hydrogels have gained great interest in the last years due to their wide range of applications from robotic and artificial muscles to drug delivery systems and biosensors. They can directly transform the electrical energy into mechanical work if placed in an electrical field. A polyelectrolyte hydrogel contains electrical charges which is bound to its polymeric network. According to the electroneutrality principle, when a charged electroactive hydrogels is placed inside a salt solution (e.g., NaCl), the unbalance between the electrical charges, causes the gel to swell. When an electrical voltage is applied to the electrodes, the local ionic strength is altered. The transient accumulation and transient depletion of mobile ions (e.g., Na^+ and Cl^-) at hydrogel and solution boundaries near the cathode side and anode side, in addition to causing swelling or shrinkage of the hydrogel-solution interfaces, create transient mechanical bending response of the electroactive hydrogel [1]. The purpose of this study is to propose and implement a numerical model for electro-actuation of the scleral tissue in support of recent experimental studies which showed that the sclera deforms when subjected to the electrical stimulations [2]. The sclera is composed of negatively charged proteoglycans and collagen fibers and we showed that it behaves like an electroactive polyanionic hydrogel. In these experiments, scleral strips were placed between two electrodes in a NaCl solution. We observed that the scleral strips bend in response to the electrical stimulations. Here, computational modelling will be used to understand and estimate the effects of various parameters on the electromechanical response of the sclera.

In the course of last decades, theoretical and computational models have been developed to study the electromechanical response of the electroactive hydrogels such as finite element models. These models are built based on principles of continuum mechanics and microscale level properties of hydrogels and their surrounding bathing fluid. In this work, we created a coupled chemo-electro-mechanical (CEM) model to investigate the electromechanical bending response of scleral tissue [3].

METHODS

Figure 1 shows the numerical representation of the experimental studies of the sclera. The scleral strips of thickness of about 1.3 mm were clamped from one side inside the 0.15M NaCl solution at the center between two electrodes 5-cm away from each other; the same dimensions were used in the numerical simulations. The nonlinear coupled Poisson-Nernst Planck (PNP) system of equations are written as:

$$\frac{\partial c_i}{\partial t} + \nabla.\left(-D\nabla c_i - z\mu F c_i \nabla \emptyset\right) = 0 \qquad (1)$$

$$\nabla^2 \emptyset = -\frac{F}{\varepsilon_0 \varepsilon_r} \sum (z_i c_i) \qquad (2)$$

where c_i is the concentration of mobile ionic species, D is diffusion constant of the ions, μ is mobility of the ionic species, R is universal gas constant, T is temperature, F is Faraday constant, $\emptyset$ is electric potential, z is the valence of the ions, ε_0 is vacuum permittivity, and ε_r is the relative permittivity of the medium. We derived the weak form equations of the PNP system by multiplying the equations in appropriate test functions and integration by parts. The resulting PNP system of equations was solved using an open-source finite element platform (FEniCS) [4]. For this purpose, GMSH software was used to generate the domains and mesh [5]. As it is shown in Figure 1, the mesh was refined near the boundaries of the sample and solution to be able to capture the steep gradient of the ion concentrations at the sample-solution interfaces.

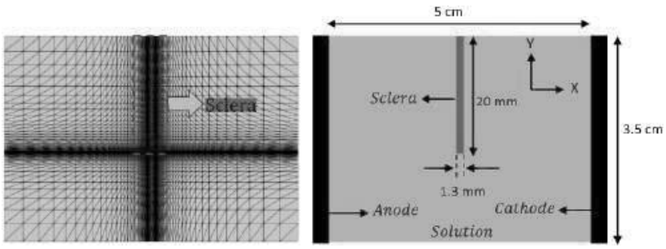

Figure 1: Illustration of the mesh and computational domains.

Furthermore, the equations of equilibrium are given by:

$$\sigma_{ij,j} + F_i = \frac{\partial^2 u_i}{\partial t^2} \qquad (3)$$

Where σ_{ij} is the stress tensor, u_i is the displacement vector, and F_i corresponds to the body force. We defined the body force by introducing the osmotic pressure:

$$\Delta\pi = RT \sum[(c_i)_{Sclera} - (c_i)_{Solution}] \qquad (4)$$

In equation 4, c_i represents the concentration of i^{th}mobile specie. Finally, the body force was defined as gradient of normalized differential osmotic pressures at the vicinity of anode side ($\Delta\pi_1$) and cathode side ($\Delta\pi_2$):

$$F_i = \frac{1}{RT} \nabla(\Delta\pi_2 - \Delta\pi_1) \qquad (5)$$

We used implicit backward Euler method to discretize the equations in time. We first validated our implementation of PNP equations in the FEniCS by reproducing the results of the reference paper [3]. The Young's modulus of the sclera, temperature, were taken equal to 0.2 MPa and 293K, respectively. The diffusion constants of the mobile ions, relative permittivity, and other constants were obtained from the literature. The simulation was performed for 60 seconds under 10 V of electrical voltage.

RESULTS

The bending angle was defined as the angle that the tip of the sample makes with respect to the initial position that was calculated in each time step. The variation of the bending angle versus time along with deformation of the tissue in time are shown in Figure 2.

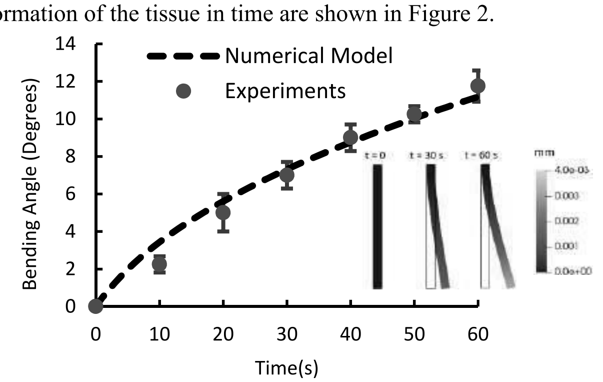

Figure 2: The numerical results of the variation of the bending angle in time are compared with the experiments. The deformation of the sample along with contour of displacement are also shown.

In this figure, the symbols show the experimental results. From fitting the model to the experimental data, the fixed charge density of 10 mM inside the tissue was found.

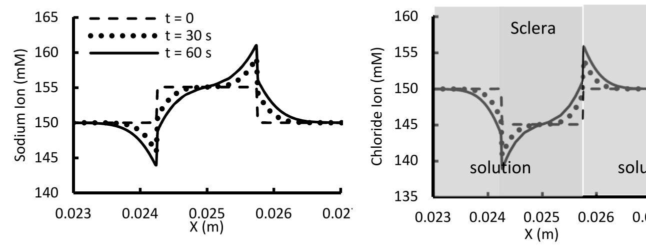

Figure 3: Concentration of the sodium (Left) and chloride (Right) ions in different times under 10V of electrical stimulation along the horizontal line

DISCUSSION

We developed and implemented a CEM model for the simulation of electroactive bending behavior of polyelectrolyte hydrogels. The focus of our study was to use this computational model for investigating the electromechanical response of the sclera.

By looking into the variation of the mobile ion concentrations in time, we observe a step-shaped of distribution of the concentration of both ions along the width of the domains before applying the electrical voltage and in equilibrium state. Once the voltage is applied, these concentrations decrease in time at the anode side (i.e., left electrode) while they increase at the cathode side (Figure 3). This is in agreement with the theory of depletion polarization [6] demonstrating the bending of the sclera to the cathode based on generation of the differential osmotic pressure at the interfaces of the sclera and solution domains.

It should be noted that we simplified this simulation to a 2D geometry in order to reduce the computational cost. However, it could be extended to a more complex 3D geometry to achieve more realistic results in future. In addition, the linear elastic material model was employed in this study for simplicity. However, the sclera is fibrous tissue and orientation of the collagen fibers plays an important role in its mechanical response. This is another important fact that we are currently working on, i.e. using a nonlinear material model for the sclera. The numerical framework of the present study could be used to estimate to model the electroactive mechanical response of both electroactive biological tissue and hydrogels.

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