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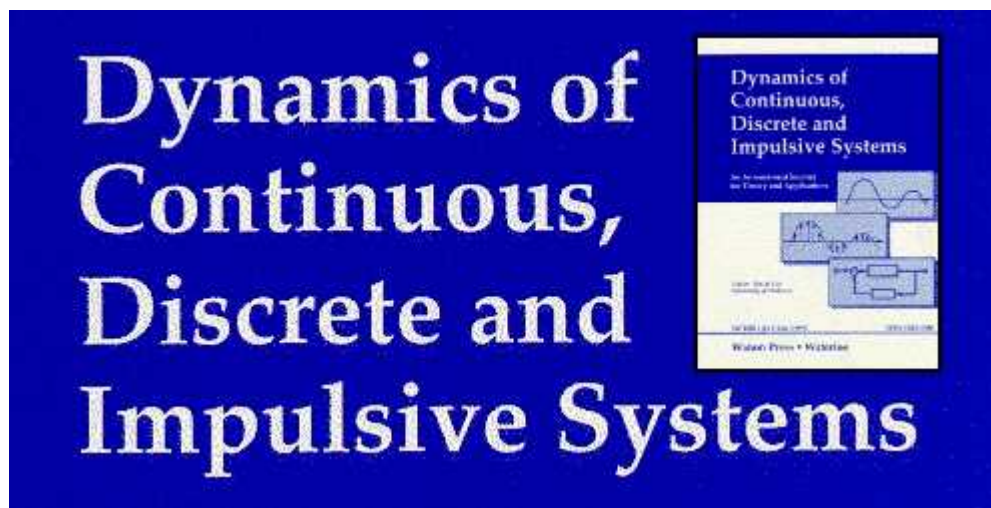
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MODELLING AND ANALYSIS OF COLLAGEN PIEZOELECTRICITY IN HUMAN CORNEA

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Abstract. This paper reports a mathematical model and finite element simulation of the dynamic piezoelectricity in human cornea including the effect of dehydration. A constitutive model is proposed for the numerical characterization of cornea based on the available experimental data in published literature. The constitutive model is then employed to derive the conservation law for the dynamic piezoelectricity supplemented by the time-dependent equation for the electromagnetic field. Electromechanical coupling in the resulting system of hyperbolic partial differential equations is treated by using the source terms. The system is solved numerically with finite element methodology. Numerical results presented here demonstrate promising applications of the developed model in aiding refractive surgery and a better understanding of regenerative processes in cornea.

Keywords. Cornea, piezoelectric, dynamics, collagen, dehydration, finite element.

1 Introduction

Cornea is one of the most delicate and active tissue systems in human and several other species. By now, we know quite a bit about the biology of this tissue system. It is a circular membrane made of mainly collagen fibers which allow transmission of the electromagnetic waves of wavelength $400 - 750nm$ with directional preference and thus protects the eye from the undesirable effect of optical scattering. Changes in the hydrated state of cornea make the system opaque. The lack of aqueous humor flow and optical absorption between the cornea and the lens can cause an increase in the intraocular pressure. This eventually may result in glaucoma. Any major change in the equilibrium stress in the sclera, zonule fibers and capillary body induce circumferential stress. Defect and perforation can cause significant change in the curvature of the cornea surfaces. Surgical process also give rise to stresses that result in change the refractive properties over time. Mathematical model and computational simulation can be useful in improving our understanding of various types of corneal defects and aid in better surgical procedures.

It may be noted that the dynamic nature of the refractive property, which is very little understood in the case of cornea as compared to the sclera, is dependent on the electrical permittivity, magnetic permeability and the piezoelectric constants of the cell-matrix composition. Complication arises because of the piezoelectricity of collagen tissue. Mechanics of collagen tissue in corneal fibroblast has been studied extensively by several researchers. Petroll *et al.*[1] studied the correlation of between the movement of cell-matrix adhesion sites and the force generation in corneal fibroblasts. A detailed discussion on the mechanism of cell regulated collagen tissue remodelling in stromal fibroblasts can be found in the paper by Girard *et al.* [2]. The experimental studies indicate a strong influence of stress-induced charge transport on the site-specific remodelling of the collagen structure in cornea. The resulting piezoelectricity is due to anisotropy of the collagen lattice [3, 4].

In cornea, stroma is the basic collagen fibril structure over which the extrafibrillar matrix is found with significant anisotropy. The cell matrix adhesion is mainly controlled by the cross-linking agent known as proteoglycans which are negatively charged. The complex structure transforms or breaks down due to change in the concentration of H_2O . Thus, the state of hydration and the anisotropy of collagen fibrils are two inter-linked and important factors that affect the piezoelectric property and hence the long-term tissue remodelling in cornea under various environmental and surgical conditions. Several important details regarding the collagen anisotropy have been reported using X-ray diffraction (see e.g. Aspden and Hukins[5]). As a fundamental cause of piezoelectricity, the structural transformation in collagen during dehydration was reported by Pratzl and Daxer [6]. Although mathematical models and computational simulations reproducing the collagen structure, as observed in the X-ray diffraction results, have been reported in a few published papers, see e.g. Pinsky *et al.*[7], not many mathematical modeling studies are found in the literature which can be applied to characterize the influence of piezoelectricity on the delicate *dynamic* activity in cornea. Experimental studies on the influence of the directional effect of the collagen structure in human cornea have been carried out in the work of Jayasuriya *et al.* [8]. These studies show a significant influence of the orientation of the collagen fibers on the stiffness and the piezoelectric coefficients of the cell-matrix composition. Furthermore, the stiffness increases and the piezoelectric constants decrease as functions of the dehydration over time. Although the related experimental investigations involve specially prepared laboratory samples, in which the mechanical state of stress and deformation are already changed compared to that in living cornea, they essentially describe the long-term behaviour of the mechanical and piezoelectric properties. Also, the anisotropic collagen structure in three dimensions is difficult to characterize experimentally and one can obtain only the correlated response using optical and X-ray measurement. Because of the above complexities, in order to provide a detailed characterization of the collagen structure and the resulting piezoelectricity, one requires comprehensive mathematical models that incorporate the important effects such as the anisotropy, the dehydration, and the small-scale dynamics of the cell-matrix adhesion.

In the present paper, we develop a mathematical model for the dynamic piezoelectricity of the corneal membrane in a continuum framework and analyze the electric polarization of the composition due to circumferential stresses acting on the cornea. The experimentally measured mechanical and piezoelectric properties reported in the work of Jayasuriya *et al.* [8] are used to construct the constitutive model. A mechanism of long-term dehydration based on the experimental observations is included in the model. Coupling between the elastodynamics and the electromagnetics is dealt with in a systematic manner. Finally, the simulated patterns of the electric field and the strain contour under circumferential stresses are demonstrated.

2 Constitutive model

Electromechanical characterization of the cornea tissue properties generally involves static and dynamic testing of samples with controlled state of dehydration and different cut angles (θ) from the cornea as schematically shown in Fig. 1. In the published literature, some results on the corneal tissue invasive measurements are available, e.g. [8]. Such measurements are made by taking into consideration the effect of the cut angle θ on the anisotropic constitutive relation. They provide further insight into orthotropic properties (stiffness and piezoelectric constants) in the plane (x, y) assuming "no out of the plane curvature". However, the collagen structure in various layers in the stroma and the type of anisotropy of the extrafibrillar structure are different. But an experimental electromechanical characterization of these differences would involve multi-axially controlled measurements which are not available at present in the published literature. Also, the site-dependence of the piezoelectric properties is most-likely influenced by the presence of fibroblasts and cell-regulated processes. This would make the constitutive model to be dependent on the high-angle X-ray data (see discussions in [7]) that reveals the structural details as some function of (x, y, z) , $z \in [h_i, h_0]$, where h_i and h_0 stand for the inner and

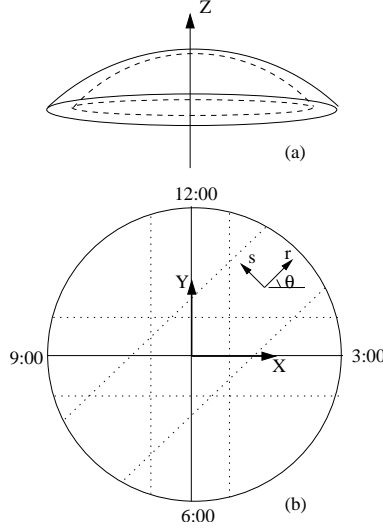


Figure 1: Schematic representation of (a) cornea model geometry and (b) angular orientation of the samples used in measuring the directional properties.

the outer surface, respectively. However, at present, due to the lack of experimental data, we have not included such details in the mathematical model. Another important aspect is the variation of the electromechanical properties as functions of dehydration over time. In our proposed constitutive model, we introduce these details at an extent available from experimental observations.

Here, we first introduce a general mathematical setting for our problem. First we define the Cartesian components of stress (σ), strain (ϵ), electric charge displacement (D), electric field intensity (E), magnetic flux (B) and the magnetic field intensity (H) in (x, y, z) . The general objective is to construct a constitutive model

$$\sigma = c\epsilon - \sigma_p(E), \quad (1a)$$

$$D = \epsilon E + P(\epsilon), \quad (1b)$$

$$B = \mu H + \mu_0 M(\epsilon), \quad (1c)$$

where c is the stiffness, σ_p is the electric polarization induced stress, ϵ is the dielectric permittivity, P is the electrical polarization vector due to transformation and deformation of the macro-molecular structure, μ is the magnetic permeability and M is the magnetic polarization vector due to molecular spin. Splitting the total charge density ρ_{total} and the total conduction current J_{total} as

$$\rho_{\text{total}} = \rho_c + \rho_p \quad (2a)$$

$$J_{\text{total}} = J + J_p + J_m, \quad (2b)$$

where ρ_c is the true charge density, ρ_p is the bound charge density, J is the true conduction current, J_p is the conduction current due to bound charge, J_m is the molecular current density, we have the local conservation laws:

$$\nabla \cdot P = -\rho_p, \quad (3a)$$

$$\nabla \times M = J_m, \quad (3b)$$

and the local continuity condition

$$\nabla \cdot \mathbf{J}_p = -\dot{\rho}_p . \quad (3c)$$

See Zhang and Li [9] for further details regarding various terms in Eqs. (2)-(3).

In order to characterize the constitutive mechanism that is likely to influence the refractive property most significantly, we consider the horizontal ($\theta = 0$), the vertical ($\theta = 90^\circ$) and the diagonal ($\theta = 45^\circ$) cuts as discussed in [8]. Dynamics of the horizontal cut sample involves (σ_{xx}, E_z) so that the longitudinal stiffness is obtained as

$$c_{11} = c_{11}^0 e^{t/\tau_1} \quad \tau_1 > 0 , \quad (4a)$$

and the piezoelectric coefficient under transverse electric polarization is obtained as

$$d_{31} = d_{31}^0 e^{t/\tau_1'} \quad \tau_1' > 0 , \quad (4b)$$

where the superscript 0 indicates the corresponding quantities at some initial state at time ($t = t_0$) and τ_n, τ_n' with $n = 1, 2, \dots$ are the times constants that are estimated from the time resolved measurements of the corresponding quantities. Similarly, for the vertical cut, which involves (σ_{yy}, E_z) , one can write

$$c_{22} = c_{22}^0 e^{t/\tau_2} \quad \tau_2 > 0 , \quad (5a)$$

$$d_{32} = d_{32}^0 e^{t/\tau_2'} \quad \tau_2' > 0 , \quad (5b)$$

With simple assumptions of aligned collagen fibers undergoing transverse electric polarization in the diagonal cut, which involves measurements in the transformed coordinate system (r, s, z) (see Fig. 1, it is reasonable to write

$$\sigma_{rr} = c_{rr} \varepsilon_{rr} - d_{3r} E_z , \quad (6a)$$

$$c_{rr} = c_{rr}^0 e^{-t/\tau_3} \quad \tau_3 > 0 , \quad (6b)$$

$$d_{3r} = d_{3r}^0 e^{-t/\tau_3'} \quad \tau_3' > 0 , \quad (6c)$$

where

$$\sigma_{rr} = \sigma_{xx} \cos^2 \theta + \sigma_{yy} \sin^2 \theta - 2\sigma_{xy} \sin \theta \cos \theta \quad (6d)$$

$$\sigma_{tt} = 0 = \sigma_{xx} \sin^2 \theta - \sigma_{yy} \cos^2 \theta - 2\sigma_{xy} \sin \theta \cos \theta \quad (6e)$$

so that the orientation-dependent properties are obtained from experiments as

$$c_{12} = (c_{rr} - c_{11}) \cot^2 \theta , \quad c_{21} = (c_{rr} - c_{22}) \tan^2 \theta , \quad (6f)$$

$$d_{36} = \frac{d_{3r} - d_{31} \cos^2 \theta - d_{32} \sin^2 \theta}{2 \sin \theta \cos \theta} . \quad (6g)$$

Note that the properties estimated in this method are the effective properties of the composition. The underlying mechanism of visco-piezoelasticity may be postulated as follows. Let us consider a representative volume element (RVE) of the cell-matrix composition and assume that the volume fraction (v_h) of the fluid phase is governed by a convection-diffusion process and can be expressed as

$$v_h = v_h^0 e^{-t/\tau_0} \quad (7)$$

and the piezoelectricity is due only to the structural transformation of the collagen fibers. Then the true charge density can be approximated as

$$\rho_c = v_h e_h , \quad (8)$$

where e_h is the specific electric dipole, Eq. (1a) takes the form

$$\boldsymbol{\sigma} = v_h \mathbf{c}_h + (1 - v_h) \mathbf{c}_f \boldsymbol{\varepsilon} - (1 - v_h) \mathbf{e}_f \mathbf{E} , \quad (9)$$

where \mathbf{c}_h is the stiffness of the fluid phase, \mathbf{c}_f is the stiffness of the oriented collagen fiber, $\mathbf{e}_f = \mathbf{e}$ denotes the electromechanical coupling coefficient matrix due to piezoelectricity in the collagen fibers. Eq. (1b) takes the form

$$\mathbf{D} = v_h \boldsymbol{\varepsilon}_h + (1 - v_h) \boldsymbol{\varepsilon}_f \mathbf{E} + (1 - v_h) \mathbf{e}^T \boldsymbol{\varepsilon} + \epsilon_0 \chi(\omega_j) \mathbf{E} , \quad (10)$$

where ϵ_0 is the dielectric constant of air, ϵ_h and ϵ_f are respectively the electric permittivity for fluid phase and the collagen fibers, $\chi(\omega_j)$ is the electric susceptibility due to the potentially active macromolecules if present in the RVE with resonant frequencies ω_j . Setting $\mathbf{M} = 0$ in Eq. (1c) leads to

$$\mathbf{B} = \mu \mathbf{H}. \quad (11)$$

In our numerical simulation we drop the above molecular susceptibility term due to unavailability of experimental data. To this end, we further simplify the general anisotropic nature of the constitutive model by neglecting certain elastic constants and certain electromechanical coupling terms, which gives finally the constitutive equations in the following matrix-vector form

$$\begin{Bmatrix} \sigma_{xx} \\ \sigma_{yy} \\ \sigma_{zz} \\ \sigma_{yz} \\ \sigma_{zx} \\ \sigma_{xy} \end{Bmatrix} = \begin{bmatrix} c_{11} & c_{12} & c_{13} & 0 & 0 & c_{16} \\ c_{21} & c_{22} & c_{23} & 0 & 0 & c_{26} \\ c_{31} & c_{32} & c_{33} & 0 & 0 & c_{36} \\ 0 & 0 & 0 & c_{44} & c_{45} & 0 \\ 0 & 0 & 0 & c_{54} & c_{55} & 0 \\ c_{16} & c_{26} & c_{36} & 0 & 0 & c_{66} \end{bmatrix} \begin{Bmatrix} \varepsilon_{xx} \\ \varepsilon_{yy} \\ \varepsilon_{zz} \\ \varepsilon_{yz} \\ \varepsilon_{zx} \\ \varepsilon_{xy} \end{Bmatrix} - \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ e_{31} & e_{32} & e_{33} & 0 & 0 & e_{36} \end{bmatrix}^T \begin{Bmatrix} E_x \\ E_y \\ E_z \end{Bmatrix}, \quad (12)$$

where

$$e_{ij} = c_{jk} d_{ik} \quad (13)$$

with Einstein's summation in tensorial index k . Having obtained an explicit form of the constitutive model, the electromechanical conservation equations are derived in the next section.

3 Dynamic piezoelectricity

The momentum conservation equation is derived in the usual manner, which is given by

$$\rho \frac{\partial^2 \mathbf{u}}{\partial t^2} - \nabla \cdot (\mathbf{c} \nabla \mathbf{u}) = \mathbf{f}(\nabla \mathbf{E}), \quad (14)$$

where the effective mass density

$$\rho = v_h \rho_h + (1 - v_h) \rho_f, \quad (15)$$

the components of the right-hand electrical source term are written as

$$f_x = -e_{31} \frac{\partial E_z}{\partial x} - e_{36} \frac{\partial E_z}{\partial y}, \quad (16a)$$

$$f_y = -e_{36} \frac{\partial E_z}{\partial x} - e_{32} \frac{\partial E_z}{\partial y}, \quad (16b)$$

$$f_z = -e_{33} \frac{\partial E_z}{\partial y}. \quad (16c)$$

We note that \mathbf{f} is a function of only the transverse electric field E_z . This is due to the particular form of electromechanical coupling assumed in Eq. (12). For practical applications, this is a reasonably simple type of electromechanical coupling, yet an important one to analyze the direct influence of piezoelectricity on the refraction of incident ray $E_z \rightarrow E_\perp$ at the outer surface $z = h_o$, with the constitutive model defined in (x, y, z) and transformed to (x, y, z_\perp) , where the subscript \perp denotes the outer surface-normal. In the finite element computation that follow, the deformations at the surfaces and at the annular base (see Fig. 1) have to satisfy the appropriate boundary conditions in a weak sense.

The transverse electric field in Eq. (16) has to satisfy Maxwell's equations for the electromagnetic field:

$$\nabla \times \mathbf{E} = -\dot{\mathbf{B}}, \quad (17a)$$

$$\nabla \times \mathbf{H} = \dot{\mathbf{D}} + \sigma_c \mathbf{E} + \mathbf{J}, \quad (17b)$$

$$\nabla \cdot \mathbf{D} = \rho_c, \quad (17c)$$

$$\nabla \cdot \mathbf{B} = 0, \quad (17d)$$

where σ_c is the effective conductivity of the RVE. The associated general impedance boundary conditions (GIBC) are

$$\mathbf{n} \times (\mathbf{E} - \mathbf{E}_\perp) = -\mathbf{J}_{sm} \quad (18a)$$

and

$$\mathbf{n} \times (\mathbf{H} - \mathbf{H}_\parallel) = \mathbf{J}_s \quad (18b)$$

at surfaces $z_\perp = h_o, h_i$, and

$$\mathbf{n} \cdot \mathbf{D} = \rho_s, \quad (18c)$$

$$\mathbf{n} \cdot \mathbf{B} = 0 \quad (18d)$$

at the annular base near the corneal anterior and scleral interface with ρ_s as the surface charge, \mathbf{n} is the unit outward surface-normal.

By using the constitutive model derived in Sec. 2, Maxwell's equations in (17a)-(17d) are combined into the following system of coupled hyperbolic equations:

$$\mu\epsilon \frac{\partial^2 \mathbf{E}}{\partial t^2} + \sigma_c \mu \frac{\partial \mathbf{E}}{\partial t} - \nabla^2 \mathbf{E} + \mu \mathbf{e}^T \frac{\partial^2 \boldsymbol{\epsilon}}{\partial t^2} - \epsilon^{-1} \nabla \nabla \cdot (\mathbf{e}^T \boldsymbol{\epsilon}) = \epsilon^{-1} \nabla \rho_c + \mu \mathbf{J}, \quad (19a)$$

$$\mu\epsilon \frac{\partial^2 \mathbf{H}}{\partial t^2} + \sigma_c \mu \frac{\partial \mathbf{H}}{\partial t} - \nabla^2 \mathbf{H} - \nabla \times (\mathbf{e}^T \frac{\partial \boldsymbol{\epsilon}}{\partial t}) = -\nabla \times \mathbf{J}, \quad (19b)$$

where the right-hand terms in Eqs. (19a)-(19b) are governed by the equation of the conduction of true charge, i.e.

$$\nabla \cdot \mathbf{J} = -\rho_c. \quad (20)$$

In the finite element simulations reported next, we have omitted the conduction part, for the sake of simplicity, while analyzing the direct piezoelectric effect. Due to this simplification, we finally have

$$\mu\epsilon \frac{\partial^2 \mathbf{E}}{\partial t^2} + \sigma_c \mu \frac{\partial \mathbf{E}}{\partial t} - \nabla^2 \mathbf{E} = \mathbf{g}^E(\partial_{tt}, \nabla, \boldsymbol{\epsilon}), \quad (21a)$$

$$\mu\epsilon \frac{\partial^2 \mathbf{H}}{\partial t^2} + \sigma_c \mu \frac{\partial \mathbf{H}}{\partial t} - \nabla^2 \mathbf{H} = \mathbf{g}^H(\partial_t, \nabla, \boldsymbol{\epsilon}), \quad (21b)$$

where the components of the right-hand source terms, which are coupled with Eq. (14), are given by

$$g_x^E = \epsilon_{11}^{-1} \frac{\partial^2 \bar{P}}{\partial x \partial z}, \quad (22a)$$

$$g_y^E = \epsilon_{22}^{-1} \frac{\partial^2 \bar{P}}{\partial y \partial z}, \quad (22b)$$

$$g_z^E = \epsilon_{33}^{-1} \frac{\partial^2 \bar{P}}{\partial z^2} - \mu_{33} \frac{\partial^2 \bar{P}}{\partial t^2}, \quad (22c)$$

$$g_x^H = \frac{\partial^2 \bar{P}}{\partial y \partial t}, \quad (23a)$$

$$g_y^H = -\frac{\partial^2 \bar{P}}{\partial x \partial t}, \quad (23b)$$

$$g_z^H = 0, \quad (23c)$$

and \bar{P} is the effective polarization (a scalar quantity) due to piezoelectricity, which is given by

$$\bar{P} = e_{31}\epsilon_{xx} + e_{32}\epsilon_{yy} + e_{33}\epsilon_{zz} + e_{36}\epsilon_{xy}. \quad (24)$$

We solve the coupled system of hyperbolic equations (14), (21a) and (21b) in $\{\mathbf{u}, \mathbf{E}, \mathbf{H}\}$ and the associated boundary conditions through three-dimensional finite element discretization of the domain shown in Fig. 1(a). A commercial package COMSOL is used in which the constitutive model and the coupled system of equations are implemented with the boundary conditions as weak constraints. Tetrahedral Lagrangian finite elements and the second order accurate time stepping scheme have been used for computation.

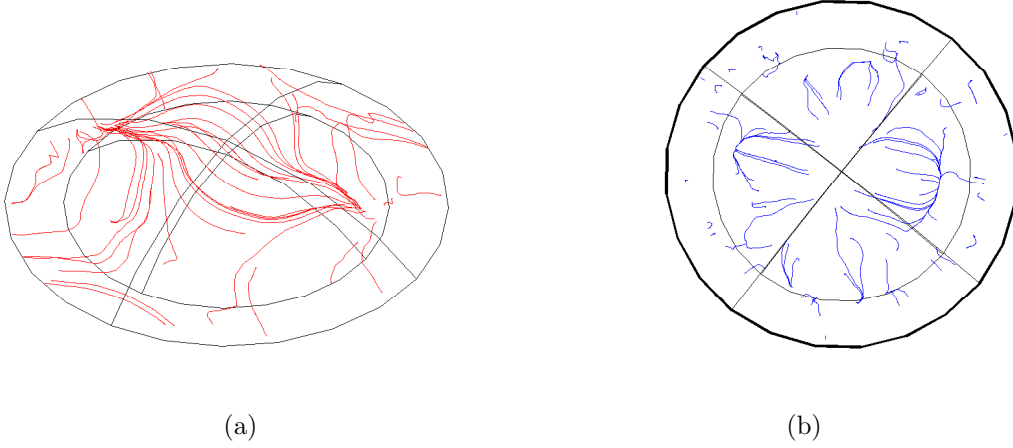


Figure 2: (a) Displacement contour (b) strain contour under harmonic stress applied at the base.

4 Computational results

We analyze a model of a (x, y) cut of the corneal section as shown in Fig. 1)(a). It contains most of the usual geometric features with inner radius $5.685mm$ and outer radius $7.259mm$. The conic-angle at the focal point is assumed to be $2 \times 59.434^\circ$ with $h_i = 2.794mm$, $h_0 - h_i = 0.449mm$ at $(x, y) = (0, 0)$. Thickness at the annular base is assumed to be $1.574mm$. A $100Hz$ harmonic stress with amplitude of $10MPa$ is applied at the base along x . The contours of displacement and the strain under the applied peak stress are shown in Fig. (2)(a) and (b), respectively. A radial pattern of the strain contour is clearly observed. Such strain distributions computed under sufficient refinement and realistically applied stresses can be helpful in a better understanding of the movement of potentially active sites of corneal fibroblasts. Further, the transverse electric field distribution, an illustration of which is shown in Fig. 3, indicates the possible regions of refractive property modification as under the applied stress. Attention has been paid to avoid the spurious effect due to mesh discretization error. The results presented here have been obtained for a refined mesh with 11987 tetrahedral elements and non-uniform time stepping set by the direct non-symmetric sparse matrix solver used. Such results may be used to analyze the post-surgical effects and also identify the location and estimate the size of the regions that are likely to undergo regenerative process due to excessive electromagnetic exposures.

5 Conclusions

A mathematical model of the dynamic piezoelectricity in human cornea has been developed. A general constitutive framework has been derived based on the available experimental results. The underlying mechanism in the cell-matrix composition that gives rise to the observed visco-piezoelectricity is discussed. The developed constitutive model has been incorporated in the time-dependent conservation laws. Finally, the coupled system of partial differential equations have been obtained and solved numerically with finite element discretization. For a model problem, typical distributions of displacements, strain, and transverse electric field have been presented and analyzed. The studies have demonstrated potential for using numerically obtained predictions in devising better surgical and tissue

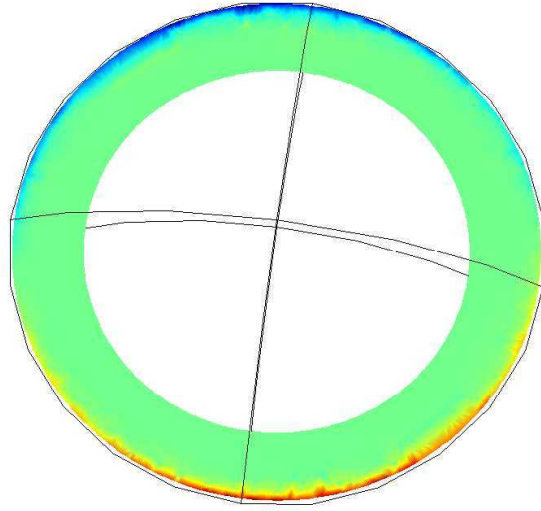


Figure 3: (a) Transverse electric field E_z at the base under harmonic stress applied at the base.

regenerative procedures.

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