Modelling aspects of the cornea (stroma)

Solid phase	Fluid phase (extrafibrillar) (no intrafibrillar fluid phase)	Bath
Collagen Proteins	Proteoglycans (charged) (negatively)	Water
	Water	Na^+
	Na^+	Cl^-
$S=\{c\}$	Cl^-	

c: collagen

Water can transfer from the F phase to to the S phase. Water and ions can move back and forth between the F phase and the Bath.

Electroneutrality in the whole medium (S+F phases)

Incompressibility of components

Mass balance and momentum balance are used for the modelling.

Incremental work done (per unit undeformed volume)

$$\delta \underset{\sim}{W} = \underset{\sim}{I} : \delta \underset{\sim}{E} + \sum_{K,\kappa \in K} \mu^{ec}_{K\kappa} \delta m^{K\kappa}$$

$\underset{\sim}{E}_G = (\underset{\sim}{F}^T \underset{\sim}{F} - \underset{\sim}{1})/2$ Green or Lagrangian strain tensor.

Several energetically conjugate stress-strain pairs

$$\underbrace{\underset{\sim}{I} : \delta \underset{\sim}{E}}_{\text{general expression}} = \underset{\sim}{\tau} : \delta \underset{\sim}{F}^T = \underset{\sim}{\underline{\tau}} : \delta \underset{\sim}{E}_G = \underset{\sim}{\tau} : \underset{\sim}{D} \delta t$$

$\underset{\sim}{\tau}$: 1st Piola-Kirchoff stress tensor

$\underset{\sim}{F}$: deformation gradient tensor

$\underset{\sim}{\underline{\tau}}$: 2nd Piola-Kirchoff stress tensor

$\underset{\sim}{D}$: rate of deformation tensor

$\underset{\sim}{\tau}$: Kirchoff stress tensor

There is no energetically conjugate strain tensor for $\underset{\sim}{\tau}$.

δt: time increment.

Relations between several stress tensors

$$\underset{\sim}{\tau} = \det \underset{\sim}{F}\ \underset{\sim}{\sigma} = \underset{\sim}{F}\cdot\underset{\sim}{\underset{\sim}{\tau}}\cdot\underset{\sim}{F}^{T} = \underset{\sim}{F}\cdot\underset{\sim}{\underset{\sim}{\Sigma}}$$

$\underset{\sim}{\sigma}$: Cauchy stress tensor (force per unit deformed area)
or
True stress

$\underset{\sim}{\Sigma}$: Force per unit undeformed area

$\underset{\sim}{\underset{\sim}{\tau}}$: Transformed force in the undeformed configuration per unit area in the undeformed configuration (no direct physical meaning)

Electrochemical potentials

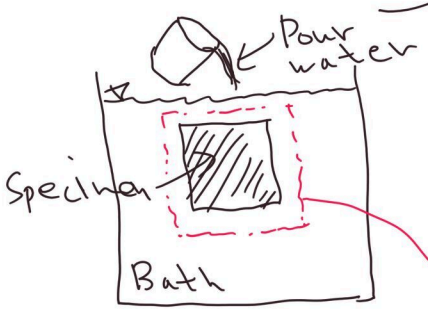
$$g^{ec}_{k\kappa} = \hat{m}_k \mu^{\circ}_{k\kappa} + \hat{v}_k P_{k\kappa} + RT \ln x_{k\kappa} + z_k F \phi_{\kappa}$$

- $\hat{m}_k \mu^{\circ}_{k\kappa}$: New element formation (enthalpy of formation)
- $\hat{v}_k P_{k\kappa}$: Mechanical part
- $RT \ln x_{k\kappa}$: Chemical (concentration) contribution
- $z_k F \phi_{\kappa}$: Electrical contribution

We may have potentials for Cl^-, due to binding of them (the Cl^-) to ligands. This triggers a chemical reaction.

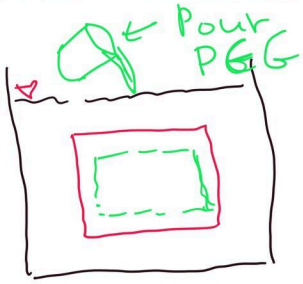
Binding of Cl^- to ligands and pH effects, cause change of electric change in the medium.

Experiment to model

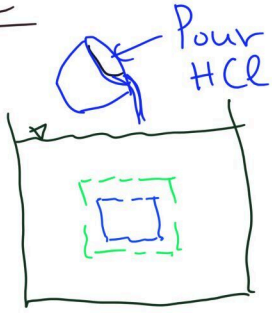


Cornea specimen in a bath.
Free swelling of the specimen.

↳ Deformed specimen



Uniform (isotropic) contraction due to osmotic pressure generated on the specimen



Contraction due to shielding of the proteoglycan repulsive forces due to the H^+.

For the mass change in the single fluid phase, we write

$$\frac{1}{\det \underset{\sim}{F}} \frac{d m^{\kappa E}}{dt} + \operatorname{div} \vec{M}_{\kappa E} = 0$$

$\vec{M}_{\kappa E}$: in-out flux of mass of conpnent κ of phase E (its the mass diffusion vector $\vec{M}$, analogous to the volume diffusion vector $\vec{J}$)

Expansion may follow dure the the increase of Cl^-, which will boost the repursive forces of the PG's.

In order to formulate the mass balance condition, we have to write appropriate growth, transfer or diffusion equations. E.g, for the whole porous medium (solid skeleton)

$$\operatorname{div} v_s + \operatorname{div} \vec{J}_E = 0$$

E: extrafibrillar phase (i.e the single fluid phase)

v_s: velocity of solid skeleton

↳ Balance of momentum

$$\operatorname{div} \underset{\sim}{\sigma} + \rho \vec{b} = \vec{0}$$

Entropy production equation, which is written as

$$\underset{\sim}{I} : \frac{d \underset{\sim}{E}}{dt} + \sum_{\kappa, \bar{\kappa}} \mu_{\kappa\bar{\kappa}} \frac{d m^{\kappa\bar{\kappa}}}{dt} \geq \frac{d W}{dt}$$

Diffusion and transfer equation

$$\vec{j} = \begin{bmatrix} \vec{J}_{wE} \\ \vec{J}_{NaE} \\ \vec{J}_{ClE} \end{bmatrix}, \quad \vec{f} = \begin{bmatrix} \vec{\nabla} g_{wE}/\vec{v}_w \\ \vec{\nabla} g^{ec}_{NaE} \\ \vec{\nabla} g^{ec}_{ClE} \end{bmatrix}$$

Relation $\vec{J}, \vec{F}$

$$\vec{J} = \underset{\sim}{K} \vec{f}$$

Chemomechanical framework (constitutive equations)

$$\underset{\sim}{T} = \frac{\partial \underline{W}}{\partial \underset{\sim}{E}}, \quad \bar{\vartheta}_{eE}^{ec} = \frac{\partial \underline{W}}{\partial N_{eE}^{*}}, \quad G_L = \frac{\partial \underline{W}}{\partial N_{ceE_L}}$$

L: ligants

$\underline{W}$ is partitioned in

1) Coupled chemomechanical contribution

$$\underline{W}_{ch\text{-}mech}\left(\underset{\sim}{E}, N_E^{*}\right)$$

($\underset{\sim}{E}$: strain; N_E^{*}: mass content)

2) Chemical contribution

$$\underline{W}_{ch}\left(E_{mo}, N_{ceE_L}\right)$$

E_{mo}: mobile costituents of the extrafibrillar phase

$$E_{mo} = \{E\} - \{PG\}$$

3) $W_{ef}\left(N_{ceE_L}\right)$ due to chemical reaction

Constitutive equations of chemo-hyperelasticity

$$\underline{W}_{ch\text{-}mech}\left(E, N_E^{*}\right) = \underset{\sim}{T}_0 : E + \underline{W}_{ch,1}\left(E, N_E^{*}\right) +$$

$$+ \underline{W}_{ch,2}\left(N_E^{*}\right)\left[\underline{W}^{gs}\left(\underset{\sim}{E}\right) + W^{c}\left(E\right)\right]$$

$\underline{W}^{gs}$: Energy of PG, other proteins

$\underline{W}^{c}$: Energy of collagen

T_0: initial stress

$$\underline{W}_{ch,1}\left(E, N_E^{*}\right) = -P_{ch}\left(N_E^{*}\right)\left(\det \underset{\sim}{F} - 1\right)$$

$\underline{W}_{ch,2}\left(N_E^{*}\right)$: amplification term