Chemoelastic energy and couplings

Form of the energy, consisting of all kinds of contributions

$$\underline{W}(\underset{\sim}{E}, E_{mo}, E_{rea}) = \underline{W}_{ch-mech}(\underset{\sim}{E}, E_{mo}) + \underbrace{\underline{W}_{ch}(E_{mo}, E_{rea}) + \underline{W}_{ef}(E_{rea})}_{\text{purely chemical part}}$$

$\underset{\sim}{E}$: strain tensor

E_{mo}: $E_{mo} = E - \{PG\}$ mass content of extrafibrillar phase, but (excluded the PG's)

E_{rea}: mass produced due to chemical reactions

E: extrafibrillar phase

Further partitions of $\underline{W}_{ch-mech}$

$$\underline{W}_{ch-mech}(\underset{\sim}{E}, E_{mo}) = W_{ch,1}(\underset{\sim}{E}, E_{mo}) + W_{ch,2}(E_{mo})\left[\underline{W}^{gs}(\underset{\sim}{E}) + \underline{W}^{c}(\underset{\sim}{E})\right]$$

$$W_{ch,1}(\underset{\sim}{E}, E_{mo}) = -p_{ch}(E_{mo})(\det \underset{\sim}{F} - 1)$$

gs: ground substance

c: collagen

Stresses in

$$gs: \underset{\sim}{T}^{gs} = \frac{\partial W^{gs}(\underset{\sim}{E})}{\partial \underset{\sim}{E}} \qquad c: \underset{\sim}{T}^{c} = \frac{\partial W^{c}(\underset{\sim}{E})}{\partial \underset{\sim}{E}}$$

Constitutive equation for the whole cartillage

$$T - T_{inc} - T_{ch} = W_{ch,2}(\underset{\sim}{T}^{gs} + \underset{\sim}{T}^{c})$$

T: ~~total~~ stress in the whole cartillage

T_{inc}: incompressibility contribution

T_{ch}: chemical contribution

In a ~~different~~ expression we can write

$$\underset{\sim}{T} + (p_E + p_{ch}) \det \underset{\sim}{F}\, \underset{\sim}{F}^{-1} \cdot \underset{\sim}{F}^{-T} = W_{ch,2}(E_{mo})\left(\frac{\partial W^{gs}(\underset{\sim}{E})}{\partial \underset{\sim}{E}} + \frac{\partial W^{c}(\underset{\sim}{E})}{\partial \underset{\sim}{E}}\right)$$

For a fictitious bath

$$\underset{\sim}{\sigma} + \hat{p}_E I + (\pi_{osm} + p_{ch}) I = W_{ch,2}(\underset{\sim}{E}_{mo})(\underset{\sim}{\sigma}^{gs} + \underset{\sim}{\sigma}^{c})$$

For the g.s.

$$\lambda = n^{gs} \Lambda_{gs}$$

λ: Lame constant of the macroscopic model

n^{gs}: porosity (volume fraction) of of g.s. in the whole medium

Λ_{gs}: the actual Lame constant of the g.s.

Similarly $\mu = n^{gs} M_{gs}$ μ: second Lamé constant.

Summary of the quantities used in the modeling of the cartilage

Set	Species	Property
E	w, PG, Na, Cl, Ca	EF compartment
E_{ions}	Na, Cl, Ca	EF ions
E_{mo}	$E - \{PG\}$	EF mobile species
I_{in}	w, Na, Ca	Independent IF species
I_{ne}	$\{w\} \cup I_{salts}$	Neutral IF species
I_{salts}	$s_1 = NaCl$, $s_2 = CaCl_2$	IF salts

Field equations (governing equations)

1) Quasi-static equilibrium: $\mathrm{div}\, \underset{\sim}{\sigma} = 0$

2) All species are incompessible

$$\mathrm{div}\, v_s + \mathrm{div}\, J_E = 0$$

s: solid skeleton

For each species (incompressibility)

$$\frac{1}{\det \underset{\sim}{F}} \frac{d v^{kE}}{dt} + \frac{1}{\det \underset{\sim}{F}} \frac{d v^{kI}}{dt} + \mathrm{div}\, J_{kE} = 0 \qquad k \in E_{ions}$$

Change of mass wrt constitutive functions

$$\frac{1}{\det F}\frac{dm^{iI}}{dt} - O_i = 0 \qquad i \in I_{in}$$

O_i: constitutive functions
For the whole medium (porous medium)

~~$O_i = O_i($~~ μ

$$\frac{1}{\det \underset{\sim}{F}}\frac{dm^{iI}}{dt} - O_i\left(\mu_{nI} - \mu_{nE}\right) = 0$$

IF mass content
$i \in I_{in}$
$n \in I_{ne}$

Chemical potentials
- For EF species
  Water: $\hat{m}_w \mu_{wE} = \hat{v}_w \underbrace{(p_{fw} + p_I)}_{p_{wE}} + RT \ln x_{wE}$ f: formation pressure
  Species K: $\hat{m}_K \mu^{ec}_{KE} = \hat{v}_K (p_{fK} + p_I) + RT \ln x_{KE} + F\zeta_K \phi_E$ $K \in E_{ions}$
- For IF species
  Water: $\hat{m}_w \mu_{wI} = \hat{v}_w (p_{adh} + p_I) + RT \ln x_{wI}$
  Similar expression for the $K \in I_{ions}$

Analogous expression for salts

Effective stress $\underset{\sim}{\sigma}'$ for the whole porous medium

$$\underset{\sim}{\sigma}' = \underset{\sim}{\sigma} + p_{eff} = \underset{\sim}{E} : \underset{\sim}{\varepsilon}$$

$\underset{\sim}{E}$: elasticity moduli for a linear constitutive equation

$\underset{\sim}{\varepsilon}$: strain tensor of collagen, $\underset{\sim}{\sigma}$: stress tensor of collagen (solid phase)

$$p_{eff} = p_I - X \qquad X: \text{chemistry dependent scalar}$$

$$X = \Lambda\left(\mathrm{tr}\,\underset{\sim}{\varepsilon} - \mathrm{tr}\,\varepsilon^{\Omega}\right) + \Pi_{osm} - p_{fw}$$

ε^{Ω}: balance pressure
Λ: chemically dependent constant

Diffusion equations

$$\vec{j} = -\underset{\sim}{K}\vec{f}$$

$$\vec{j} = \begin{bmatrix} J_{wE} \\ J_{NaE} \\ J_{CaE} \\ J_{ClE} \end{bmatrix}, \qquad \vec{f} = \begin{bmatrix} \rho_w \vec{\nabla}\mu_{wE} \\ \rho_{Na}\vec{\nabla}\mu^{ec}_{NaE} \\ \rho_{Ca}\vec{\nabla}\mu^{ec}_{CaE} \\ \rho_{Cl}\vec{\nabla}\mu^{ec}_{ClE} \end{bmatrix}$$

$\underset{\sim}{K}$: diffusion coefficient matrix

Energetically conjugate quantities and associated phenomena

Phenomenon	Generalised strain	Generalized stress
Chemoelasticity	ε of porous medium	σ total stress
Osmosis (coupled)	m^{wE}	μ_{wE}
Chemomechanical coupling	m^{iE}, $i \in E_{in}$	μ_{nE} $n \in E_{salts}$
Seepage, electroosmosis	J_{wE}	$e_w \vec{\nabla} \mu_{wE}$
Ions	J_{kE}	$e_k \vec{\nabla} \mu^{ec}_{kE}$
Transfer through collagen fibers	m^{iI}, $i \in I_{in}$	$\mu_{nI} - \mu_{nE}$ $n \in I_{ne}$

in: independent species