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A 3-D Model for Finite Viscoelastic Swelling of Charged Tissues and Gels

Materials like soft biological tissues undergo large viscoelastic deformations during the swelling process. Following this, it is the goal of this contribution to merge the advances of finite viscoelasticity laws and the state of the art in electrochemical swelling theories within a well-founded multiphasic concept. The numerical treatment is carried out fully 3-d in the framework of the FEM.

1. Multiphasic formulation for charged tissues and gels by the Theory of Porous Media

The Theory of Porous Media (TPM) is a macroscopic continuum theory which is based on the theory of mixtures and the concept of volume fractions. For more details see [1] and citations therein. Proceeding from a binary mixture consisting of solid and fluid constituents φ^α denoted by $\alpha = \{S, F\}$, the solid phase is extended by incorporating the volume free fixed charges φ^{fc} . Furthermore, the interstitial fluid φ^F is assumed to be composed of three components φ^β , namely the liquid solvent, the cations and the anions, indicated by $\beta = \{L, +, -\}$. By introducing the volume fractions $n^\alpha = dv^\alpha/dv$, the saturation constraint yields

$$\sum_{\alpha} n^{\alpha} = n^S + n^F = 1, \quad \text{where} \quad n^F = n^L + n^+ + n^-. \quad (1)$$

The model under consideration incorporates seven independent fields: the solid displacement \mathbf{u}_S , the seepage velocity \mathbf{w}_F , the relative ion velocities \mathbf{w}_γ , the entire pore-fluid pressure p and the molar ion concentrations c_m^γ , where $\gamma = \{+, -\}$ indicates only the mobile ion constituents. For the liquid solvent it is assumed that $\dot{\mathbf{x}}_S \approx \dot{\mathbf{x}}_L$, i. e., $\mathbf{w}_L \approx \mathbf{w}_F$. Herein, $(\cdot)'_\alpha$ denotes the material time derivative with respect to φ^α . Proceeding from materially incompressible constituents without any mass exchanges due to chemical reactions, volume balances for the constituents φ^α , concentration balances for the components φ^β and the quasi-static momentum balances are introduced:

$$(n^\alpha)'_\alpha + n^\alpha \operatorname{div} \dot{\mathbf{x}}_\alpha = 0, \quad (n^F c_m^\beta)'_\beta + n^F c_m^\beta \operatorname{div} \dot{\mathbf{x}}_\beta = 0 \quad \text{and} \quad \mathbf{0} = \operatorname{div} \mathbf{T}^\alpha + \rho^\alpha \mathbf{b} + \hat{\mathbf{p}}^\alpha. \quad (2)$$

Furthermore, $\mathbf{T}^\alpha = (\mathbf{T}^\alpha)^T$ are the symmetric partial *Cauchy* stress tensors, $\rho^\alpha \mathbf{b}$ represent the body forces and $\hat{\mathbf{p}}^\alpha$ are the momentum productions, where $\hat{\mathbf{p}}^S + \hat{\mathbf{p}}^F = \mathbf{0}$ must hold due the overall conservation of momentum.

2. Constitutive equations for the multiphasic model

Proceeding from the effective stress principle, cf. [1], the following relations hold:

$$\mathbf{T}^\alpha = -n^\alpha \mathcal{P} \mathbf{I} + \mathbf{T}_E^\alpha, \quad \hat{\mathbf{p}}^F = \mathcal{P} \operatorname{grad} n^F + \hat{\mathbf{p}}_E^F. \quad (3)$$

Herein, the *Lagrangian* multiplier \mathcal{P} maintains the incompressibility condition. Additionally, for the so-called extra quantities $(\cdot)_E$, some further constitutive assumptions are needed. From thermodynamical considerations, it follows that

$$\mathbf{T}_E^\alpha = -n^\alpha \sum_{\beta} \mu_F^\beta \mathbf{I} + \mathbf{T}_{E \text{ mech.}}^\alpha \quad \text{and} \quad \hat{\mathbf{p}}_E^F = \sum_{\beta} \mu_F^\beta \operatorname{grad} n^F - \frac{(n^F)^2 \gamma^{FR}}{k^F} \mathbf{w}_F. \quad (4)$$

Therein μ_F^β are the electrochemical potentials of φ^β per fluid volume [J/m^3] and $\mathbf{T}_{E \text{ mech.}}^\alpha$ is the purely mechanical part of \mathbf{T}_E^α , where $\mathbf{T}_{E \text{ mech.}}^S$ is computed from an appropriate viscoelasticity law [2,3] and, *a priori*, $\mathbf{T}_{E \text{ mech.}}^F \approx \mathbf{0}$. Moreover, γ^{FR} is the effective fluid weight and k^F denotes the *Darcy* permeability. Following this, one can introduce the entire (hydraulic and osmotic) fluid pressure as $p = \mathcal{P} + \sum_{\beta} \mu_F^\beta$. For the chemical equations, the molar electrochemical potentials [J/mol] of the fluid components are needed which are given by

$$\mu_m^L = \mu_{m0}^L + R\theta \ln \frac{c_m^L}{\sum_{\beta} c_m^\beta}, \quad \mu_m^\gamma = \mu_{m0}^\gamma + R\theta \ln c_m^\gamma + z^\gamma F \xi. \quad (5)$$

These terms are related to μ_F^β via $\mu_m^\beta = \mu_F^\beta / c_m^\beta$. Moreover, μ_{m0}^β are the initial chemical potentials of the components, R is the universal gas constant, θ is the absolute *Kelvin*'s temperature, z^γ are the valences of the ions, F is the *Faraday* constant and ξ is the electrical potential.

3. Interstitial fluid flow, ion diffusion and osmotic pressure

The interstitial fluid flow can be described by an extended *Darcy* filter law and the ion diffusion by an extended

Nernst-Planck equation [4]:

$$n^F \mathbf{w}_F = -\frac{k^F}{\gamma^{FR}} (\text{grad } \mathcal{P} - \rho^{FR} \mathbf{b} + \sum_{\beta} \text{grad } \mu_F^{\beta}), \quad c_m^{\gamma} \mathbf{w}_{\gamma} = -D^{\gamma} [\text{grad } c_m^{\gamma} + z^{\gamma} c_m^{\gamma} \frac{F}{R\theta} \text{grad } \xi] + c_m^{\gamma} \mathbf{w}_F. \quad (6)$$

Herein, $n^F \mathbf{w}_F$ is the filter velocity and $c_m^{\gamma} \mathbf{w}_{\gamma}$ is the relative ion velocity, wherein $c_m^{\gamma} \mathbf{w}_F$ is added to the ion velocity to obtain the ion velocity relative to the solid motion.

The osmotic pressure π is calculated from the osmolarity difference of the internal and external solutions:

$$\pi = R\theta [(c_m^+ + c_m^-) - (\bar{c}_m^+ + \bar{c}_m^-)]. \quad (7)$$

Note that the concentration of the fixed charges does not appear in this equation, since φ^{fc} is regarded as a part of the solid meshwork.

4. Numerical treatment of the governing equations

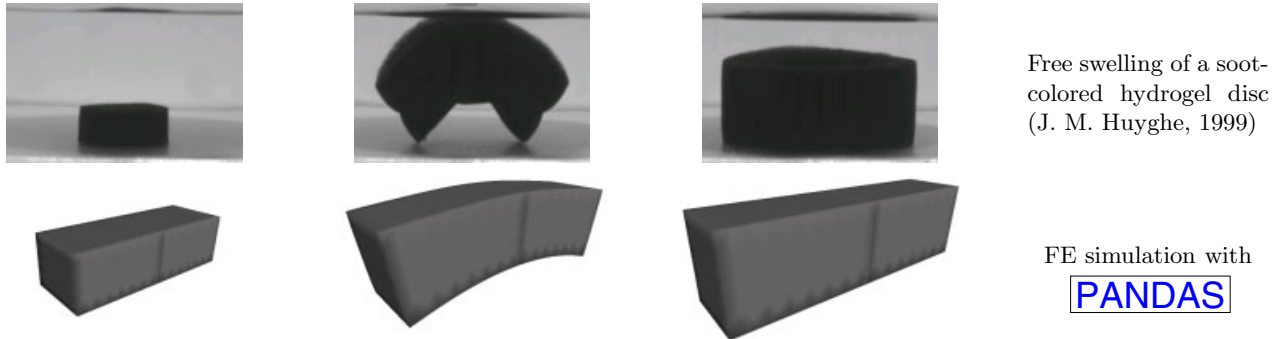
For the numerical treatment, the electroneutrality condition $z^+ c_m^+ + z^- c_m^- + z^{fc} c_m^{fc} = 0$ with the valences $z^+ = 1$, $z^- = -1$ and $z^{fc} = -1$ of a monovalent solution is used, so that the gradient of the electrical potential can be calculated by [5]

$$I = FA (c_m^+ \mathbf{w}_+ - c_m^- \mathbf{w}_-) = \mathbf{0}. \quad (8)$$

Furthermore, the balance relations are weighted by independent test functions and after integration over the spatial domain Ω with the surface $\partial\Omega$ one obtains a displacement-pressure-concentration formulation in the primary variables \mathbf{u}_S , p and c_m . For more details, cf. [3].

5. Examples: Free swelling of a hydrogel block

To demonstrate the capability of the presented model, a free swelling experiment on hydrogel is simulated by the FEM. Therefore, a 3-d block is discretized with hexagonal extended *Taylor-Hood* elements with a quadratic approximation of \mathbf{u}_S and linear approximations of p and c_m . To initiate swelling, the concentration of the external solution was decreased from 0.15 mol/l to 0.125 mol/l within 10 sec.



6. References

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