THEORY AND NUMERICS OF MULTICOMPONENT MIXTURE MODELS FOR SOFT BIOLOGICAL TISSUES

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Summary One natural category of porous materials is represented by biological soft tissues, such as cartilage, lung or skin. The challenge of describing these materials lies in their complex inhomogeneous microstructure consisting of mostly ionized water and collagen fibers embedded in an extracellular meshwork of charged protein compounds. In order to describe the physiological behaviour of soft tissues on the macroscale, the electro-chemomechanical couplings between the constituents as well as the viscoelastic and anisotropic properties of the extracellular matrix must be considered. In order to meet these requirements, the well-founded Theory of Porous Media (TPM) is applied, which consistently allows for the description of multiphasic continua with internal interactions. For the efficient numerical treatment within the FEM, the governing set of multi-field equations is rewritten in weak form including physically meaningful boundary terms. The overall applicability of the multicomponent mixture approach is finally shown by representative numerical examples.

INTRODUCTION

Currently, most models that describe the electro-chemomechanical behaviour of soft biological tissues are restricted either to small strains or to finite but purely elastic skeleton deformations. Moreover, anisotropic and inhomogeneous properties are, in general, not considered. In fact, these types of naturally grown materials undergo large viscoelastic deformations, where the extracellular matrix exhibits so-called intrinsic viscoelastic properties [2]. These flow-independent viscoelastic effects are strongly coupled with the dissipative phenomena resulting from the interstitial fluid flow and the electrochemical (osmotic and electrostatic) swelling mechanisms [5, 6]. Furthermore, their inner structure and thus, the associated physical properties are inhomogeneously distributed over the 3-d anatomic shape of the tissue. In addition, anisotropic properties may occur due to embedded collagen fibers and orientation-dependent hydraulic and electrolytic conductivities.

The goal of this contribution is to present a consistent theoretical framework based on the Theory of Porous Media (TPM), where the constitutive assumptions, necessary to cover all relevant tissue properties, are merged in a modular manner. This actually allows for a concise representation of the resulting system of coupled partial differential equations, which can be efficiently treated within the finite element method (FEM) and thus, enables the numerical solution of even large 3-d problems at suitable computational costs.

MULTICOMPONENT MIXTURE MODEL

The TPM is a macroscopic continuum theory, which is based on the theory of mixtures extended by the concept of volume fractions [1]. 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 $\beta = \{L,\, +,\, -\}$ (figure 1). Assuming materially incompressible constituents, the volume fractions $n^\alpha = \mathrm{d}v^\alpha/\mathrm{d}v$ (partial volume v^α per bulk volume v) serve as describing physical quantities consistent with the saturation constraint $\sum_\alpha n^\alpha = 1$. In addition, the molar concentrations $c_m^\beta = \mathrm{d}n_m^\beta/\mathrm{d}v^F$ (moles n_m^β per fluid volume v^F) are introduced as the describing quantities of the ionic components. Note that the chemical potentials can be used, alternatively [4].

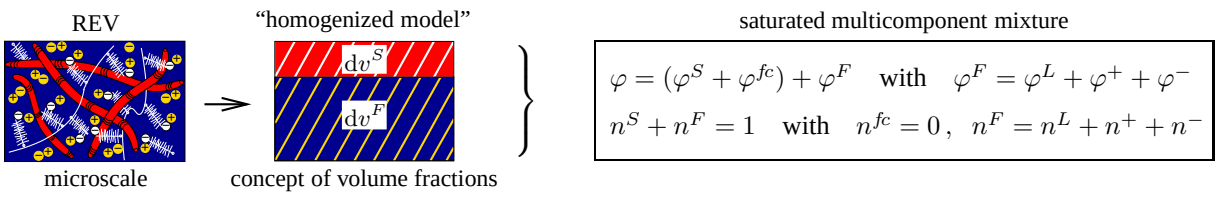

Figure 1: *Multicomponent TPM model of charged hydrated tissue*

Following the idea of superimposed continua [1], each component follows its individual motion $\mathbf{x} = \boldsymbol{\chi}_\alpha(\mathbf{X}_\alpha, t)$ and has its own velocity field $\overset{\prime}{\mathbf{x}}_\alpha = \mathrm{d}\boldsymbol{\chi}_\alpha(\mathbf{X}_\alpha, t)/\mathrm{d}t$ with respect to different reference positions $\mathbf{X}_\alpha$. Therein, $(\,\cdot\,)'_\alpha$ denotes the material time derivative following the motion of φ^α. Thus, the model under consideration incorporates seven independent fields, namely the solid displacement $\mathbf{u}_S = \mathbf{x} - \mathbf{X}_S$, the seepage velocity $\mathbf{w}_F = \overset{\prime}{\mathbf{x}}_F - \overset{\prime}{\mathbf{x}}_S$, the relative ion velocities

$\mathbf{w}_\gamma = \overset{\prime}{\mathbf{x}}_\gamma - \overset{\prime}{\mathbf{x}}_S$, the effective interstitial fluid pressure p, and the molar ion concentrations c_m^γ, where $\gamma = +, -$ indicates only the mobile ions. Note that the fixed charges are directly coupled to the solid displacement and thus, represent no independent field. Moreover, for the liquid solvent, it is assumed that $\overset{\prime}{\mathbf{x}}_L \approx \overset{\prime}{\mathbf{x}}_F$, i. e. $\mathbf{w}_L \approx \mathbf{w}_F$.

GOVERNING EQUATIONS

For the numerical treatment within the FEM, weak forms of the governing multi-field equations are required. Therefore, the seepage velocity and the cation diffusion are eliminated by use of the extended *Darcy* filter law and the extended *Nernst-Planck* equation. Together with the electroneutrality condition, this yields a concise representation of the governing balance relations by means of the primary variables $\mathbf{u}_S$, p, and c_m^+. Subsequently, weighted by independent test functions and integrated over the spatial domain Ω with the surface $\partial\Omega$, one finds the respective weak form of the mixture volume (MV), the cation concentration (CC), and the mixture momentum (MM) balances:

$$\mathcal{G}_{\mathrm{MV}} \equiv \int_\Omega \delta p \,\mathrm{div}\,(\mathbf{u}_S)'_S \,\mathrm{d}v - \int_\Omega \mathrm{grad}\,\delta p \cdot n^F \mathbf{w}_F \,\mathrm{d}v + \int_{\partial\Omega} \delta p\, \bar{q}\,\mathrm{d}a = 0\,,$$

$$\mathcal{G}_{\mathrm{CC}} \equiv \int_\Omega \delta c_m^+ \left[\, n^F (c_m^+)'_S + c_m^+ \,\mathrm{div}\,(\mathbf{u}_S)'_S \,\right] \mathrm{d}v - \int_\Omega \mathrm{grad}\,\delta c_m^+ \cdot n^F c_m\, \mathbf{w}_+ \,\mathrm{d}v + \int_{\partial\Omega} \delta c_m^+\, \bar{\jmath}\,\mathrm{d}a = 0\,,$$

$$\mathcal{G}_{\mathrm{MM}} \equiv \int_\Omega \mathrm{grad}\,\delta\mathbf{u}_S \cdot (\mathbf{T}^S_{E\,\mathrm{mech.}} - p\,\mathbf{I}\,)\,\mathrm{d}v - \int_{\partial\Omega} \delta\mathbf{u}_S \cdot \bar{\mathbf{t}}\,\mathrm{d}a = 0\,.$$

Therein, $\delta\mathbf{u}_S$, δp, and δc_m^+ are the corresponding test functions, $\bar{q}$ denotes the efflux of the interstitial fluid over the surface $\partial\Omega$, $\bar{\jmath}$ is the anion diffusion over $\partial\Omega$, and $\bar{\mathbf{t}}$ is the external load vector acting on the entire mixture. Moreover, $\mathbf{T}^S_{E\,\mathrm{mech.}} = \mathbf{T}^S_{EQ} + \mathbf{T}^S_{NEQ} + \mathbf{T}^S_{ANISO}$ represents the purely mechanical *Cauchy* extra stress tensor, which is constitutively decomposed into isotropic elastic (equilibrium) and viscoelastic (non-equilibrium) parts $\mathbf{T}^S_{EQ}$ and $\mathbf{T}^S_{NEQ}$, as well as an anisotropic term $\mathbf{T}^S_{ANISO}$. Note that the hydraulic and osmotic stress contributions are completely included in the entire fluid pressure p.

NUMERICAL EXAMPLES

The efficiency of the presented model is shown by two fully coupled 3-d simulations using the FE tool PANDAS. By incorporating appropriate constitutive equations for the description of the osmotic and electrostatic phenomena [3], it is possible to simulate free swelling behaviour. For the example depicted in the left hand side of figure 2, the external ion concentration was lowered on the yellow surrounding surface to initiate swelling. Furthermore, the model can be applied for the description of intervertebral disc (IVD) tissue, whenever the implemented constitutive law for $\mathbf{T}^S_{ANISO}$ is suitable for the macroscopic simulation of the collagen fiber-bundles within the anulus fibrosus. First physically sound results are achieved on an idealized 3-d geometry of a motion segment of the lumbar spine subjected to an axial compressive load yielding a finite deformation response of the IVD (figure 2 right).

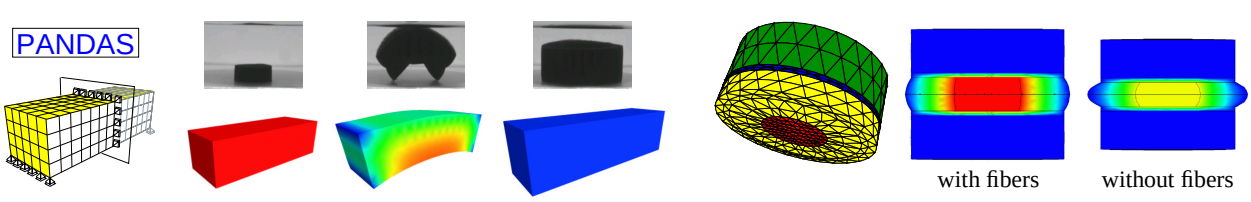

Figure 2: *Free swelling of a hydrogel block (left) and idealized model of the IVD with nucleus pulposus and anulus fibrosus (right)*

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