SIMULATION OF THE COUPLED STRUCTURAL-TRANSPORT RESPONSE OF SOFT TISSUE STRUCTURES USING FINITE ELEMENT MODELS

Bruce R. Simon (1), Stuart K. Williams (2), Zun P. Liu (1), and Paul H. Rigby (2)

(1) Aerospace and Mechanical Engininneering Department
(2) Biomedical Engineering Interdisciplinary Program
The University of Arizona
Tucson, Arizona

INTRODUCTION

Soft tissue structures and associated tissue engineered (TE) materials can be studied using models based on porous media/mixture theories in which multiple charged mobile species are dissolved in a mobile fluid (*f*) that saturates the "pores" in a highly deformable "solid" fibrous matrix (*s*) in which fixed charge is present—represented by fixed charge density (FCD). This class of analysis has been utilized for various biological structures including arterial tissue [1], articular cartilage [2], and TE constructs [3]. Finite element models (FEMs) have been developed for the study of these complex problems. Current theoretical models identify various forms for the material properties that can be measured. Here these properties are identified and related mathematically so that they may be utilized in various FEMs. Examples are given to illustrate the effects of finite strain and material properties in FEMs of soft tissue structures.

THEORY

The continuum formulations can be Eulerian or Lagrangian for quasi-static, finite straining of anisotropic materials with no body forces. For clarity, consider three charged mobile species, denoted by $\alpha, \beta = p\,(+),\ m\,(-),\ b\,(\pm)$ that are dissolved in an incompressible fluid (water) with concentration, $c^\alpha = dn^\alpha / dV^f$ or $\tilde{c}^\alpha = Jnc^\alpha$ and valence z^α. Assuming the solid is incompressible and saturated by the fluid, the porosity, $n = dV^f / dV = 1 - J^{-1}(1-n_0)$ where $n_0 = dV_0^f / dV_0 = n_0(X_i)$ is the initial (measured) porosity. The FCD, $c^F = dn^F / dV^f$ or $\tilde{c}_0^F = dn^F / dV = Jnc^F = \tilde{c}_0^F(X_i)$, i.e. the initial (measured) FCD. Electroneutrality requires that $\Sigma_\alpha z^\alpha nc^\alpha + c^F = 0$ and an electrical potential, μ^e will develop or can be applied to the material. The displacements, solid velocity, and relative fluid/species velocites are $u_i = x_i - X_i$, $\mathrm{v}_i = \dot{u}_i = \mathrm{v}_i^s$, and $\mathrm{v}_i^{\gamma r} = n(\mathrm{v}_i^\gamma - \mathrm{v}_i^s)$ with $\gamma, \delta = f, p, m, b$. The deformation gradient, $F_{ij} = \partial x_i / \partial X_j$; volumetric strain, $J = dV / dV_0$; Green's strain, $E_{ij} = 1/2\,(F_{ki}F_{kj} - \delta_{ij})$; and Finger's strain, $H_{ij} = F_{ik}^{-1}F_{jk}^{-1}$. The total stress (Cauchy), σ_{ij} is related to the solid stress, σ_{ij}^s and fluid stress, $\sigma_{ij}^f = -p^f\delta_{ij}$ (hydrostatic fluid pressure, p^f), as $\sigma_{ij} = (1-n)\sigma_{ij}^s - np^f\delta_{ij}$. Relative species flux $j_i^{fr} = \mathrm{v}_i^{fr}$ and $j_i^{\alpha r} = c^\alpha \mathrm{v}_i^{\alpha r}$. The relative electrical flux (current density), $j_i^{er} = i_i^{er} = \Sigma_\alpha F_c z^\alpha j^{\alpha r}$. The mixed models are based on continuous "primary" fields u_i and generalized potentials $\mu^{\gamma *}, \nu^{\xi *}$, etc. (see below) that are continuous; whereas the "secondary" fields p^f, μ^e, and c^α may be discontinuous at material interfaces. The Eulerian phenomenological equations are a basis for all models beginning with the

MIX (Mixture) Model

$$\bar{\mu}_{xi}^{\bar{\xi}} = \Sigma_{\bar{\eta}} f_{ij}^{\bar{\xi}\bar{\eta}}(\mathrm{v}_j^{\bar{\eta}} - \mathrm{v}_j^s), \quad (\bar{\xi}, \bar{\eta} = s, f, p, m, b)$$

$$\bar{\mu}_{xi}^s = [(1-n)\sigma_{ji}^s]_{,j} + n_{,j}\sigma_{ji}^f - (1-n)\rho_T^s \bar{\mu}^s_{,i}, \quad \bar{\mu}_{xi}^f = [n\sigma_{ji}^f]_{,j}$$

$-n_{,j}\sigma_{ji}^f - n\rho_T^f \bar{\mu}^f_{,i}$; and $\bar{\mu}_{xi}^\alpha = -nc^\alpha M^\alpha (F_c z^\alpha \mu^e + \mu^\alpha)_{,i}$ with material properties: $f_{ij}^{\bar{\xi}\bar{\eta}} = f_{ji}^{\bar{\eta}\bar{\xi}}$; $f_{ij}^{\bar{\xi}\bar{\eta}} = 0$, $\bar{\xi} \neq \bar{\eta}$. Introducing definitions of total stress and relative velocities yields the

PM (Porous Media) Model

$$\sigma_{ji,j} = 0, \quad -n^2 c^\gamma \bar{\mu}_{,i}^{\gamma *} = \Sigma_\delta\, a_{ij}^{\gamma\delta} \mathrm{v}_j^{\delta r}; \quad (\gamma, \delta = f, p, m, b)$$

with properties: $a_{ij}^{ff} = f_{ij}^{fs} + \Sigma_\alpha f_{ij}^{f\alpha}$, $a_{ij}^{f\alpha} = a_{ij}^{\alpha f} = -f_{ij}^{f\alpha}$, etc. Now solve for relative flux in the last two PM equations and introduce the relative flux definitions to obtain

MPMT (Mixed Porous Media Transport) Model.

$$\sigma_{ji,j} = 0, \quad j_i^{\gamma r} = -\Sigma_\delta L_{ijM}^{\gamma\delta} \mu_{,j}^{\delta *}$$

with properties: $L_{ijM}^{ff} = n^2 \hat{a}_{ij}^{ff}$, $L_{ijM}^{f\alpha} = L_{jiM}^{\alpha f} = n^2 c^\alpha \hat{a}_{ij}^{\alpha f}$, etc. where $\hat{a}^{\alpha\beta} = [a^{\alpha\beta}]^{-1}$. The total fluid pressure/potential, $\mu^{f*} = p^f + p^o$ and the electro-chemical potentials $\mu^{\alpha *} = F_c z^\alpha \mu^e + \mu^\alpha$ are given in terms of osmotic pressure $p^o = p_0^o - RT\Sigma_\alpha \phi^\alpha c^\alpha$ and chemical potential $\mu^\alpha = \mu_0^\alpha + RT\, ln(\gamma^\alpha c^\alpha)$ to formulate the

PMT (Porous Media Transport) Model.

Again $\sigma_{ji,j} = 0$ and now the generalized (Eulerian) Darcy law is

$$v_i^{fr} = -k_{ij}^{ff}[p_{,j}^f + \sum_\alpha (\sum_\beta b_{jk}^{f\beta} c^\beta \frac{\partial \mu^\beta}{\partial c^\alpha} c_{,k}^\alpha + \delta_{jk} \frac{\partial p^0}{\partial c^\alpha} c_{,k}^\alpha + b_{jk}^{f\alpha} c^\alpha F_c z^\alpha \mu_{,k}^e)\,]$$

Fick's law is $j_i^{\alpha r} = -\sum_\beta d_{ij}^{\alpha\beta} c_{,j}^\beta - d_{ij}^{\alpha e} \mu_{,j}^e + b_{ij}^{\alpha f} c^\alpha v_j^{fr}$. The material property functions are the hydraulic permeability, $k_{ij}^{ff} = n^2 (a_{ij}^{ff} - \Sigma_\alpha a_{im}^{f\varepsilon} \Sigma_\beta \hat{a}_{mn}^{\alpha\beta} a_{nj}^{\beta f})^{-1}$; the chemical and electrical diffusivities, $d_{ij}^{\alpha\beta} = \Sigma_\beta \ell_{ij}^{\alpha\gamma} \frac{\partial \mu^\gamma}{\partial c^\beta} \neq d_{ji}^{\beta\alpha}$ and $d_{ij}^{\alpha e} = \Sigma_\beta F_c z^\beta \ell_{ij}^{\alpha\beta}$ (with $\ell_{ij}^{\alpha\beta} = nc^\alpha \hat{a}_{ij}^{\alpha\beta} c^\beta n = \ell_{ji}^{\beta\alpha}$) and generalized convection coefficients $b_{ij}^{\alpha f} = \Sigma_\beta \hat{a}_{ik}^{\alpha\beta} a_{kj}^{\beta f} = b_{ji}^{f\alpha}$. The PMT properties are related to $L_{ijM}^{\gamma\delta}$ as $L_{ijM}^{ff} = k_{ij}^{ff}$, etc. Note that ABAQUS FEMs are based on an Eulerian view of the material as a porous hyperelastic material (PHE) that is saturated by an incompressible mobile fluid with no mobile species.

EMPMT (Electrical Mixed Porous Media Transport) Model.

Iintroducing relative current as one flux in $j_i^{\xi r} = \Sigma_\gamma T_M^{\xi\gamma} j_i^{\gamma r}$ and modified potentials defined as $\nu^{\xi *} = \Sigma_\delta T_M^{\delta\xi} \mu^{\delta *}$ (with non-zero terms $T_M^{ff} = T_M^{mm} = T_M^{bb} = 1$, $T_M^{\alpha e} = F_c z^\alpha$ and $\xi, \eta = f, e, m, b$) in the MPMT model, $\sigma_{ji,j} = 0$ and $j_i^{\xi r} = -\Sigma_\eta L_{ijE}^{\xi\eta} \nu_{,j}^{\eta *}$ where $L_{ijE}^{\xi\eta} = \Sigma_\gamma \Sigma_\eta T_M^{\xi\gamma} L_{ijM}^{\gamma\delta} T_M^{\eta\delta}$.

Lagrangian EMPMTS MODEL. The field theory includes the conservation laws $T_{ji,j} = 0$ $(T_{ji} = F_{ik} S_{jk},\ S_{ij} = JF_{im}^{-1} \sigma_{mn} F_{jn}^{-1})$ and $\tilde{Q}^\xi + \tilde{j}_{k,k}^{\xi r} = 0$; $\tilde{Q}^f = \dot{J}$, $\tilde{Q}^e = 0$, $\tilde{Q}^m = \dot{\tilde{c}}^m$, $\tilde{Q}^b = \dot{\tilde{c}}^b$; constitutive equations, e.g. "effective" stress $S_{ij} = S_{ij}^{eff} - Jp^f H_{ij}$ and $\tilde{j}_i^{\xi r} = -\Sigma_\eta \tilde{L}_{ijE}^{\xi\eta} \tilde{\nu}_{,j}^{\eta *}$, $\tilde{L}_{ijE}^{\xi\eta} = JF_{ik}^{-1} L_{kmE}^{\xi\eta} F_{mj}^{-1}$. Electroneutrality is $\Sigma_\alpha z^\alpha \tilde{c}^\alpha + \tilde{c}_0^F = 0$. Material properties are S_{ij}^{eff} and $\tilde{L}_{ijE}^{\xi\eta}$ that can represent various materials, e.g. for TE materials, S_{ij}^{eff} may take the form for a stiff crushable foam (e.g. ePTFE scaffolds). Compliant materials (e.g. arteries) may be hyperelastic with $S_{ij}^{eff} = \partial U^{eff} / \partial E_{ij}$, e.g. "Fung's" exponential form, $U^{eff} = U^{eff}(\varphi) = C_0(e^\varphi - 1)$, $\tilde{L}_{ijE}^{\xi\eta} = \tilde{L}_{ijE}^{\xi\eta}(\varphi)$, and $\varphi = \varphi(E_{ij}, J, n, \tilde{\nu}^{\xi *}, T)$.

FINITE ELEMENT MODELS

Lagrangian EMPMT FEMs are based on elemental interpolations $u_i = N_N^u \bar{u}_{Ni}$, $u_{i,j} = N_{N,j}^u \bar{u}_{Ni}$, $\tilde{\nu}^{\xi *} = N_M^\xi \bar{\nu}_M^{\xi *}$, $\tilde{\nu}_{,j}^\xi = N_{M,j}^\xi \bar{\nu}_M^\xi$. Galerkin residuals are $\psi_{Ni}^u = \int N_{N,j}^u T_{ji} dV_0 - \int N_N^u \sigma_{ji} \hat{n}_j dA = 0$ and $\psi_M^\xi = -\int N_M^\xi \tilde{Q}^\xi dV_0 - \int N_{M,k}^\xi \tilde{j}_k^{\xi r} dV_0 - \int N_M^\xi j_k^{\xi r} \hat{n}_k dA = 0$ that are assembled, boundary/initial conditions imposed, a time integrator applied, and a transient solution for the primary fields is obtained using iterative predictor-corrector algorithms. Iteration is also used to determine the secondary fields (p^f, μ^e, c^α) at the Gauss points in each finite element.

REPRESENTATIVE RESULTS

An ABAQUS FEM of a large arterial wall was used to predict the relative fluid flux at various pressures in the cardiac cycle. Figure 1 shows fluid flux (at P = 120 mm Hg) that is significantly different from fluid flux associated with constant pressure, indicating a complex convection transport field in the wall during cyclic pressurization.

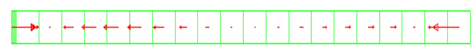

Figure 1. ABAQUS FEM of Arterial Wall Fluid Flux

Figure 2 shows the development of the concentration field for a single neutral species in a 1D EMPMT FEM where large strains greatly reduce the porosity and cause the concentrations to be markedly increased (due to reductions in the amount of fluid).

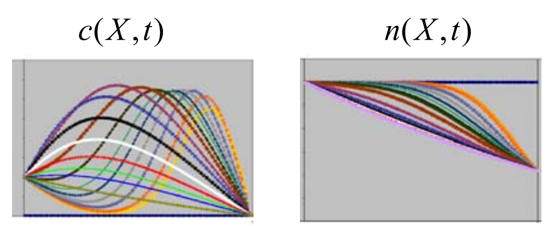

Figure 2. EMPMT FEM of Concentration and Porosity

These and other examples demonstrate the capability of these FEMs based on mixed PMT models to simulate coupled structural-transport in complicated biological structures where finite strain occurs. These procedures are currently being used to study vascular wall mechanics and the design of TEVGs including structural response and species transport.

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