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Short Communication

Determination of poroelastic properties of cartilage using constrained optimization coupled with finite element analysis

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ABSTRACT

The feasibility of determining biphasic material properties using a finite element model of stress relaxation coupled with two types of constrained optimization to match measured data was investigated. Comparison of these two approaches, a zero-order method and a gradient-based algorithm, validated the predicted material properties. Optimizations were started from multiple different initial guesses of material properties (design variables) to establish the robustness of the optimization. Overall, the optimal values are close to those found by Cohen et al. (1998) but these small differences produced a marked improvement in the fit to the measured stress relaxation. Despite the greater deviation in the optimized values obtained from the zero-order method, both optimization procedures produced material properties that gave equally good overall fits to the measured data. Furthermore, optimized values were all within the expected range of material properties. Modeling stress relaxation using the optimized material properties showed an excellent fit to the entire time history of the measured data.

1. Introduction

Articular cartilage is the bearing surface in freely movable joints. As a load bearing tissue, the mechanical properties of articular cartilage are important indicators of its ability to perform its intended functions, and methods for measuring its mechanical properties have been developed over the past 30 years. Cartilage is often modeled using biphasic or poroelastic theories, which simulate the coupled interactions between the porous solid skeleton and the mobile tissue fluid (Mow et al., 1980; Armstrong et al., 1984).

Typically, mechanical properties are estimated by fitting a constitutive model to experimental data. Depending on the complexity of the constitutive model and experimental configuration, the relationship between the model and experiment might be expressed as an algebraic equation, the solution of a differential equation or as a computational model. For example, the isotropic and transversely isotropic properties of cartilage have been determined by fitting solutions of differential equations of biphasic material models to stress relaxation data (Mow et al., 1980; Cohen et al., 1998). In these cases material properties were determined by minimizing the squared difference

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between measured and predicted load intensity. Poroelastic rather than biphasic models are commonly used for computational models of cartilage since they are easily accessible in commercially available finite element (FE) codes such as ABAQUS, ANSYS, COMSOL, etc. However, Simon (1992) showed that the linear biphasic and poroelastic theories are related mathematically through a transformation of kinematic variables.

In the past 20 years, computational models have played a more prominent role in the prediction of material properties from experimental data. Computational models are particularly attractive for implementing complex tissue models such as those with fiber reinforcement, spatially varying properties, hyperelastic or viscoelastic properties (Oomens et al., 1993; Cohen et al., 1994; Wilson et al., 2004; Lei and Szeri, 2007; Liu and Ovaert, 2011; Seifzadeh et al., 2012; Fu et al., 2013; Yao et al., 2014; Reutlinger et al., 2014). Using an FE model integrated with optimization routines, material properties can be found by minimizing the squared difference between simulated and measured results such as force, stress or displacement. Diverse optimization algorithms have been used. For example, the mean values of hyperelastic properties of liver tissue were quantified using Levenberg–Marquardt optimization and verified using Monte-Carlo methods (Fu et al., 2013), and Liu and Ovaert (2011) used a differential evolution algorithm combined with a poroviscoelastic FE model to estimate viscoelastic properties of hydrogels in creep. Recently, Reutlinger et al. (2014) obtained the optimized material parameters of intervertebral disc that minimized the error between simulated displacement and experimental displacement after the bounds on hyperelastic parameters were implemented in the particle swarm optimization. In all of the examples cited above, the optimization was unconstrained. Constraints were not imposed on acceptable values of material properties or on the fit of measured to computed responses, i.e., stress or displacement. In addition, the robustness of the convergence to a set of material properties was, in general, not investigated in all these investigations. Wilson et al. (2004) determined the fibril-reinforced poroviscoelastic material properties of cartilage with depth-dependent collagen orientation by fitting the reaction force and lateral displacement of the numerical results to the corresponding experimental values, but they did not provide evidence for a unique fit using different initial values of the material properties between lower and upper bounds. However some exceptions include Lei and Szeri (2007), who showed that the history of aggregate modulus converged although they did not show the convergence history of the four other material properties with different initial guesses. Seifzadeh et al. (2012) predicted the material properties of human cartilage using a fibril-reinforced poroviscoelastic model coupled with a simulated annealing algorithm (MATLAB), which searched for the robustness of optimization using several initial guesses. In each of the aforementioned investigations the optimization was unconstrained.

The aim of this investigation was to evaluate the feasibility of using constrained optimization to determine the material properties of a transversely isotropic porous elastic material from measured stress relaxation data. Optimization was performed using two different approaches: (a) a zero-order method, which is available in ANSYS, and (b) a gradient-based solver in SmartDO, which interfaces with ANSYS via Tcl/Tk.

2. Methods

Our previously developed and validated transversely isotropic poroelastic model of unconfined compression stress relaxation (Chung and Mansour, 2013) was coupled with constrained optimization procedures. Experimental stress relaxation data for unconfined compression of growth plate were obtained from Cohen et al. (1998), who used unconstrained optimization to predict biphasic material properties ($E_t = 4.3$ MPa, $E_a = 0.64$ MPa, $\nu_t = 0.49$, $\nu_{at} = 0$ and $k = 5\times10^{-15}\,\mathrm{m^4N^{-1}s^{-1}}$) where the tissue was loaded at a constant strain rate of $7.6\times10^{-4}\,\mathrm{s^{-1}}$ to 10% strain.

Constitutive relations for a linear anisotropic poroelastic material can be constructed following the generalized Hooke's law (Detournay and Cheng, 1993; Simon, 1992; Cheng, 1997)

$$\sigma_{ij} = D_{ijkl}\varepsilon_{kl} - \alpha_{ij}p \tag{1}$$

$$p = K_m(\zeta - \alpha_{ij}\varepsilon_{ii}) \tag{2}$$

Eq. (1) is the constitutive response for the porous solid, where D_{ijkl} is an elastic modulus tensor of the solid skeleton, ε_{kl} is a total elastic strain tensor, and p is the pore fluid pressure. For a transversely isotropic material D_{ijkl} has five independent material constants (Chung and Mansour, 2013) whereas for an isotropic material D_{ijkl} has two independent material constants and the Biot coefficient tensor, α_{ij}, degenerates into a scalar, i.e., $\alpha_{ij} = \alpha\delta_{ij}$ where δ_{ij} is a second-order unit tensor. Eq. (2) is the constitutive response for the pore fluid, where K_m is the Biot modulus, ζ is the volumetric fluid strain, and ε_{ii} is the elastic volumetric strain which is the trace of the strain tensor.

The slow transport of fluid in porous media is governed by Darcy's law

$$q_i = -\kappa_{ij}(\nabla p - f_i) \tag{3}$$

where q_i is the fluid mass flow rate, κ_{ij} is a second-order permeability tensor, and f_i is the fluid body force per unit volume.

In general, a constrained optimization problem is formulated as follows: find a vector of design variables $\{X\} = \{x_1, x_2, \cdots\cdots, x_n\}$ that minimizes the objective function $F(\{X\})$ subject to inequality constraints on the state variables $S_i^L \le S_i(\{X\}) \le S_i^U$, $i = 1, 2, \cdots\cdots, m$, and the lower and upper bounds on the design variables $x_k^L \le x_k \le x_k^U$, $k = 1, 2, \cdots\cdots, n$, where n is the number of design variables, and m is the number of state variables which are the response of the design.

To implement the optimization procedures, the design variables were the transversely isotropic material properties $\{X\} = \{E_t, E_a, \nu_t, \nu_{at}, k\}$. Lower and upper bounds on the first three design variables were set as

$$3.34\ \mathrm{M\ Pa} \le E_t \le 5.76\ \mathrm{MPa} \tag{4}$$

$$0.36\ \mathrm{M\ Pa} \le E_a \le 0.59\ \mathrm{MPa} \tag{5}$$

$$0.1 \le \nu_t \le 0.49 \tag{6}$$

as in Table 1 of Cohen et al. (1998). Bounds on permeability

$$1.8\times10^{-15}\,\mathrm{m^4N^{-1}s^{-1}} \le k \le 5.0\times10^{-15}\,\mathrm{m^4N^{-1}s^{-1}} \tag{7}$$

were set from data in Villemure and Stokes (2009), as was the out of plane Poisson's ratio;

$$0.01 \le \nu_{at} \le 0.1 \tag{8}$$