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Evaluation of hyperelastic models for the non-linear and non-uniform high strain-rate mechanics of tibial cartilage

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ABSTRACT

Accurate modeling of the high strain-rate response of healthy human knee cartilage is critical to investigating the mechanism(s) of knee osteoarthritis and other cartilage disorders. Osteoarthritis has been suggested to originate from regional shifts in joint loading during walking and other high strain-rate physical activities. Tibial plateau cartilage under compression rates analogous to walking exhibits a non-linear and location-dependent mechanical response. A constitutive model of cartilage that efficiently predicts the non-linear and non-uniform high strain-rate mechanics of tibial plateau cartilage is important for computational studies of osteoarthritis development. A transversely isotropic hyperelastic statistical chain model has been developed. The model's ability to simulate the 1-strain/s unconfined compression response of healthy human tibial plateau articular cartilage has been assessed, along with two other hyperelastic statistical chain models. The transversely isotropic model exhibited a superior fit to the non-linear stress–strain response of the cartilage. Furthermore, the model maintained its predictive capability after being reduced from four degrees of freedom to one. The remaining material constant of the model, which represented the local collagen density of the tissue, demonstrated a regional dependence in close agreement with physiological variations in collagen density and cartilage modulus in human knees. The transversely isotropic eight-chain network of freely jointed chains with a regionally-dependent material constant represents a novel and efficient approach for modeling the complex response of human tibial cartilage under high strain-rate compression. The anisotropy and microstructural variations of the cartilage matrix dictate the model's response, rendering it directly applicable to computational modeling of the human knee.

1. Introduction

Deterioration of knee articular cartilage (AC) leads to severe joint debilitation in the form of osteoarthritis (Buckwalter et al., 2005). Identifying the mechanism(s) that causes healthy AC to degenerate into this diseased state is of high priority. While computational knee models enable the systematic and controlled evaluation of potential osteoarthritis disease mechanisms (Wilson et al., 2005), the utility of these models' results relies on the accuracy of the modeled AC.

Articular cartilage poses a modeling challenge due to its complex physiology and equally complex mechanical response. It consists of a solid phase of cartilage cells (chondrocytes) embedded within an extracellular matrix and a fluid phase of water and soluble ions (Poole et al., 2001). The extracellular matrix is composed mainly of cross-linked type II collagen fibrils and negatively charged proteoglycan macromolecules. The interaction of the solid and fluid phases creates a non-linear poroviscoelastic response to compressive loading (Mow et al., 1984). Extensive work has been done to model this behavior (Boschetti et al., 2006; Hayes et al., 1972; Lai et al., 1991; Mak, 1986; Wilson et al., 2004). The short-term, high strain-rate response of AC, however, depends predominantly on the flow-independent, intrinsic viscoelasticity of the matrix (Bader and Kempson, 1994), which results from the collagen meshwork and its entrapment of high-swelling aggrecan macromolecules (Maroudas, 1976). The collagen network in the superficial tangential zone (STZ) is particularly important in the tissue's response to high-rate loading (Mizrahi et al., 1986). These data suggest that the mechanical response of knee AC to high-rate loading (e.g., walking) (Liu et al., 2010) may be represented by using the collagen meshwork and its anisotropy as the main input parameters. This unique approach would afford representation of the non-linear elastic response of AC with a low number of

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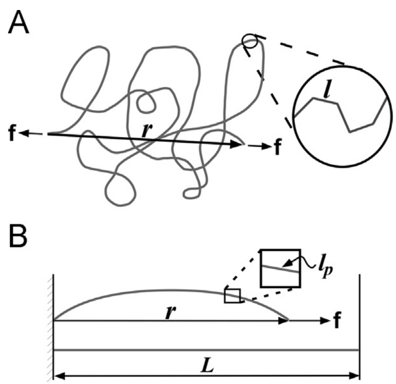

Fig. 1. Schematics of the two statistical chain models used to model tibial cartilage. The application of tension, f, stretches the chain to vector length r. (A) The highly flexible freely jointed chain, composed of N rigid links of length l. (B) The semi-flexible MacKintosh chain with contour length L and persistence length l_p. Adapted from Palmer and Boyce (2008).

material constants to facilitate implementation in a whole-joint computational model.

The structural properties of the STZ are non-uniform across the tibial plateau, which in turn may promote heterogeneous mechanical properties. The regions of the plateau covered by meniscal tissue, for example, tend to have a thicker STZ, more tangentially oriented collagen fibrils, and a higher collagen density, compared to regions not covered by meniscal tissue (Clark, 1991; Eyre et al., 2006). Individual collagen fibrils are primarily tensile elements. Thus when the collagen network is compressed, fibrils oriented perpendicular to the loading axis will stretch and resist the deformation, while fibrils oriented parallel to the loading axis will provide minimal load support. Therefore, regions with large amounts of tangentially oriented collagen fibrils, such as meniscus-covered regions, are expected to exhibit larger compressive stiffness compared to other regions, which has been supported experimentally (Barker and Seedhom, 2001; Shepherd and Seedhom, 1999; Young et al., 2007). The regional variability, however, may be more complex; we recently demonstrated that AC elastic moduli beneath the external and posterior portions of the menisci exceeded 300% of AC not covered by the meniscus and of AC beneath the anterior third of the menisci (Deneweth et al., 2013). Insight into knee AC behavior and the development of osteoarthritis, therefore, appear better served by modeling both the non-linear and non-uniform elastic response of the STZ.

Statistical mechanics models offer the ability to predict finite deformations of hyperelastic materials with relatively few material constants (Boyce and Arruda, 2000). These mechanistic models are particularly powerful because they offer insight into the underlying physiological factors driving mechanical behaviors (Ma et al., 2010). A material is represented as a cross-linked network of flexible molecular chains (Arruda and Boyce, 1993). The chains, which can be analogized to "entropy springs," produce significant forces when stretched but have minimal resistance to compression, much like collagen fibrils. As the material is deformed, the chains rotate and stretch to accommodate the deformation, altering the statistical entropy of the chain network and producing network stress.

Statistical mechanics models have accurately modeled multiple finite deformation states in elastic polymers (Boyce and Arruda, 2000; Boyce et al., 1994) and, more recently, in biological materials (Bischoff et al., 2004; Ma et al., 2010; Palmer and Boyce, 2008). Since the driver of knee AC short-term response, the collagen network, can be analogized to a statistical chain network, these models are strong candidates for modeling the short-term response of AC (Brown et al., 2009). However, the ability of the model to replicate the high strain-rates associated with walking or the non-uniform mechanical properties of tibial AC remains unknown. The purpose of this study, therefore, was two-fold. Firstly, the aim was to determine which, if any, of three popular statistical mechanics models could successfully model unconfined axial compression behavior of tibial AC, and secondly, to determine the extent to which the model that best fit the data could capture the regional mechanical properties of the tissue.

2. Methods

Statistical mechanics models have two key components: the mathematical description of the chains and the manner in which the chains are assembled to form a network. Two chain models, the freely jointed chain (FJC) model (Kühn and Grun, 1942) and the MacKintosh chain (MAC) model (MacKintosh et al., 1995), were each implemented within an isotropic eight-chain network (Arruda and Boyce, 1993; Palmer and Boyce, 2008). Additionally, the freely jointed chain was placed in a transversely isotropic eight-chain network (Bischoff et al., 2002) to develop a third model (TI). These three models were applied to experimental data from a series of unconfined axial compression tests of healthy human proximal tibial AC (Deneweth et al., 2013). The model that was found to best approximate the experimental data was further examined to determine the extent to which its parameters manifested regional dependence similar to that identified experimentally.

2.1. Freely jointed chain

The freely jointed chain is a highly flexible unconstrained rotating chain comprised of N rigid segments of length l positioned in three-dimensional space to give an initial chain vector length r_0 (Fig. 1a) (Kühn and Grun, 1942). The chain is highly flexible such that $r_0 \ll Nl$. Tension in the chain at length r is:

$$f_{FJC} = \frac{k\Theta}{l}\frac{r}{Nl}\frac{\left(3-\left(\frac{r}{Nl}\right)^2\right)}{\left(1-\left(\frac{r}{Nl}\right)^2\right)} \tag{1}$$

where k is Boltzmann's constant, 1.38065×10^{-23} J K^{-1}, and Θ is the absolute temperature.

2.2. MacKintosh chain

The MacKintosh chain describes a semi-flexible statistical chain with significant bending rigidity. The length of the chain over which it appears straight, that is, its persistence length l_p, is approximately equal to its contour length L (Fig. 1b) (MacKintosh et al., 1995). The chain exhibits an average end-to-end resting length r_0 and an average vector length under no applied tension $r_{f=0}$. L, l_p, and $r_{f=0}$ are related by (Palmer and Boyce, 2008):

$$r_{f=0} = L\left(1-\frac{L}{6l_P}\right) \tag{2}$$

The tension developed in the chain when it is extended to an end-to-end length r can be written as:

$$f_{chain} = \frac{k\Theta}{l_p}\left(\frac{1}{4(1-r/L)^2}\right)\left(\frac{L/l_p-6(1-r/L)}{L/l_p-2(1-r/L)}\right) \tag{3}$$

2.3. Isotropic eight-chain network (FJC and MAC)

The isotropic eight-chain network treats a unit cell of material as a cube with sides aligned along the principal axes of stretch (Fig. 2) (Arruda and Boyce, 1993). Eight chains originate from the center of the cube and extend to each corner. Incorporating Eq. (1) into the isotropic eight-chain network yields the strain energy, U_{FJC}, for the FJC model:

$$U_{FJC} = nk\Theta N\left\{\frac{\lambda_{chain}}{\sqrt{N}}\beta_{chain} + \ln\frac{\beta_{chain}}{\sinh\beta_{chain}}\right\} \tag{4}$$

where n is the chain density, $\lambda_{chain} = (\lambda_1{}^2+\lambda_2{}^2+\lambda_3{}^2)^{1/2}/\sqrt{3}$, λ_i is the principal stretch in the ith direction (i=1, 2, 3), and β_{chain} is the inverse Langevin ($\mathscr{L}^{-1}$) of $\lambda_{chain}/\sqrt{N}$ (Arruda and Boyce, 1993).

Cartilage behaves as a nearly incompressible material under high strain-rates (Wong et al., 2000) and is frequently modeled as incompressible (Ateshian et al., 2007; Brown et al., 2009; Mow et al., 1980). For unconfined compression of an incompressible material, employing the Padé approximation of the inverse Langevin (Cohen, 1991), the nominal stress in the axial direction becomes (Arruda and Boyce, 1993):

$$T_{o1FJC} = \frac{nk\theta}{3}\frac{\sqrt{N}}{\lambda_{chain}}\mathscr{L}^{-1}\left(\frac{\lambda_{chain}}{\sqrt{N}}\right)(\lambda-1/\lambda^2) \tag{5}$$