Modeling Nutrient Transport Coupled with Mechanics in Tendon Fibers

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Self-assembly of biomolecules is a promising avenue towards the development of new materials. Biological tissues serve as model factories for the production of macromolecular structures, where the processes of molecular self-assembly and macroscopic growth are integrated in robust systems. Growth occurs as nutrients, amino acids, and enzymes undergo mass transport and react to increasing tissue mass. At the molecular scale, there is considerable understanding of the reactions for self-assembly of tissue components such as collagen. There is less understanding of the thermodynamic driving forces and of how these interact with growth processes to form multicellular tissue. These processes are also influenced by mechanics at the continuum scale. Here, we present a study of the processes of self-assembly and growth of tendon fibers from the fibrillar to the continuum scale. At the continuum scale, we have developed a mixture theory that couple the mechanical deformation and growth (mass increase) of the solid phase (representing the collagen fibrils) the transport of the interstitial fluid phase, and the diffusion of solutes (representing the precursors and byproducts of growth) dissolved in the fluid phase. The constitutive relations for the flux of the fluid and solutes are developed following thermodynamic arguments. In a generalization of Darcy's Law, the fluid flux is related through the permeability to the driving force that includes the inertial and body forces of the solid phase and gradient in fluid partial pressure. The driving force for solute diffusion is computed from the gradient of the chemical potential. We assume a simple model for the chemical potential and recover the volume-averaged transport equation for solute dispersion in a porous-media flow. Specifically, the contribution of diffusion to the solute flux is related to the concentration gradient through the dispersion tensor. At the fibril scale, permeabilities as a function of the fibril packing are determined by direct fluid flow simulations using the Lattice Boltzmann (LB) method. For the solute transport, the dispersion tensor is determined as a function of the Peclet number by simulating dispersion at the fibril-scale using finite differences and the flow field obtained from the LB simulations.