A chemo-mechanical model for hydrogel gelation: coupling of fluid swelling, crosslinking shrinkage and reactive-diffusive mechanisms

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ABSTRACT

Recent 3D bioprinting technology allows us to print three-dimensional scaffolds where living cells are embedded in biocompatible materials. Due to its biocompatibility, intelligent behaviour and relatively low cost, alginate hydrogel is a natural polymer which has been extensively used as bio-ink for the production of scaffolds for cell growth, division, and reproduction. Alginate hydrogel undergoes mild gelation by adding an ionic stimulus (cross-linker), such as Calcium which stabilizes the polymer network via cross-linking [1]. The gelation process is promoted by the diffusion of the solvent and the onset of chemical reactions in the hydrogel [2]. This process will also produce inelastic deformation, in turn, responsible for residual stresses and will affect the structural resolution, shape fidelity, final scaffold geometry and the cell behaviour inside the biomaterial. This work aims to develop a computational model of the gelation mechanism in alginate hydrogels. The chemo-mechanical system consists of elastic, shrinking and swelling mechanical deformations promoted by the chemical potentials of the cross-linker and the fluid content. The constitutive model explicitly accounts for the influence of the cross-linker and the fluid on the inelastic deformation gradients associated with shrinking and swelling phenomena. The developed computational framework allows to quantitatively predict the heterogeneous gelation and stress distribution inside the hydrogel as a function of internal chemical reactions [3,4,5]. Numerical approaches for multiphysics mechanisms have been developed and implemented in a finite element framework, considering the monolithic coupling of chemical transport and mechanics [6]. The benchmark test validates the computational framework which is calibrated towards experimental data. The importance of the coupling effect between shrinking and swelling phenomena is highlighted, showing the effectiveness of the model and the potential impact on bioprinting applications.

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