Numerical implementation of a coupled diffusion-deformation theory for polymeric structures

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ABSTRACT

A dry polymer network is a three dimensional network of long cross-linked polymers which has flexible chains and allows for large chain deformation. Swelling occurs when a dry polymer solid enters a humid environment and absorbs water molecules [1]. Swelling polymers are globally used in diverse applications including carriers for drug delivery, actuators and sensors in microfluidic devices, biosensors, contact lenses, disposable diapers and processed food. There is a need to understand the swelling and disintegration of multi-component polymeric structures such as immediate and controlled release tablets. The swollen disintegrant particles in the tablet increase stress, thus weakening the tablet structure. Finally, the tablet disintegrates and the active substance is released in the desired manner. Modelling of a swelling polymeric matrix involves concurrent deformation of the polymer network and diffusion of the solvent through the network. This study will contribute with an understanding of the mechanical behaviour of the polymer release matrix. A continuum-mechanical theory to describe the various coupled aspects of fluid permeation and large deformation (e.g., swelling) of polymeric matrix has been implemented. The basic mechanical force balance laws and the balance law for the fluid content are reviewed. The main purpose of this paper is to discuss the details of numerical implementation of coupled diffusion-deformation theory for a polymeric matrix. The theory is developed by considering thermodynamically consistent, large-deformation and continuum-mechanical laws to describe the mutual interaction of mechanics and chemistry for solids capable of absorbing fluid-like chemical species. Special constitutive equations are discussed with limitation to isotropic materials, and free energy model based on a Flory-Huggins model for the energy change due to mixing of the fluid with the polymer network, coupled with a non-Gaussian statistical-mechanical model for the change in configurational entropy which accounts for the limited extensibility of polymer chains. The fluid-solid mixture is treated as a single homogenized continuum body which allows for a mass flux of the solid [2], [3]. The theory has been implemented numerically using finite difference method (FDM) in MATLAB code and ABAQUS CAE 6.14-1 Finite Element commercial software for solving coupled diffusion-deformation boundary value problems for polymeric matrix. As representative examples of application of the theory, this study shows: (a) three-dimensional swelling-equilibrium of a polymeric matrix in an unconstrained, stress-free state; and (b) one-dimensional transient problems: free-swelling of a polymeric matrix. The numerical results are compared with the existing experimental results.

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