Multiphysics Modeling of Swelling Gels

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Abstract

Introduction: Polymer gels are elastic materials consisting of a network of cross-linked polymers swollen with a fluid, generally a liquid solvent, which are subject to large volume deformations (swelling/shrinking) as a consequence of the change in solvent content [1]. Thus, modeling swelling processes involves the coupled solvent migration and large elastic deformations of the polymer network. Some species of gels are also able to respond to particular non-mechanical stimuli, like temperature or pH changes, varying their swelling degree. Current applications of gels include food industry, coating and printing processes, microfluidic devices (pumps and valves), cosmetics and medicines. In particular, in biomedical applications gels are commonly employed as controlled drug release devices. Moreover, many biological tissues are made of gels. The growing interest in these systems require theoretical and computational models capable of accurately predicting the swelling dynamics, in order to eventually improve the design of devices for technological applications. Use of COMSOL Multiphysics: In order to analyze the dynamics of swelling gels, we set a three-dimensional non-linear theoretical and numerical model which couples solvent diffusion and large elastic deformations [2]. The numerical model is implemented in COMSOL Multiphysics 4.2a using the Weak Form PDE interface. In dealing with the volume constraint which relates the volume change with the solvent content, we adopt a mixed approach with a suitable choice of the shape functions for the state variables of the problem. Moreover the non-linear boundary conditions expressing the chemical equilibrium on the boundary of the gel are implemented through a 2D weak form algebraic equation defined on the boundary of the 3D domain. The possibility of defining surface physics on boundaries of 3D domains is crucial for our modeling approach. Results: The numerical model is employed to carry out several numerical simulations in which the transient behavior of gels with different geometries and boundary conditions is involved [2]. Through these simulations we are able to show interesting deformation patterns and test the robustness of the model. In Figure 1 one frame of the transient free-swelling of a cubic gel sample immersed in a solvent bath is shown: note that, due to the non-homogeneous swelling, the shape of the sample is not cubic during the transient, as the corners and the edges, having a larger contact surface with the solvent, swell first with respect to the faces. Conclusion: we have successfully implemented and solved a system of coupled non-linear PDEs describing the concurrent solvent diffusion and large deformations which characterize swelling gels. The model is successfully benchmarked through several numerical experiments. Future directions include the simulation of surface instability phenomena, like wrinkling and creasing, which are among the most attracting deformation patterns that can be observed in swelling gels and are object of recent research in controlling surface properties and in shape morphing techniques [3].

Reference

1. M. Doi, Gel Dynamics, Journal of the Physical Society of Japan, 78, 052001 (2009).
2. A. Lucantonio et al., Transient analysis of swelling-induced large deformations in polymer gels, submitted (2012).
3. S. Yang et al., Harnessing Surface Wrinkle Patterns in Soft Matter, Advanced Functional Materials, 20, 2550-2564 (2010).

Figures used in the abstract

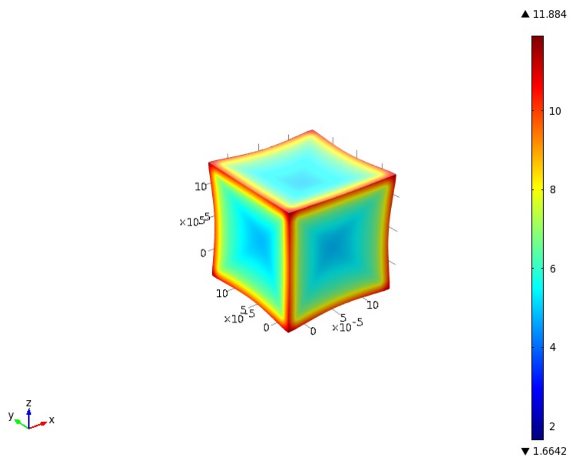

Figure 1: One frame of the transient free-swelling of a cubic gel sample; color-code refers to the swelling ratio with respect to the initial volume of the cube.