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A multiplicative finite element algorithm for the inhomogeneous swelling of polymeric gels

Yin Liu, Hongwu Zhang[1], Yonggang Zheng*

State Key Laboratory of Structural Analysis for Industrial Equipment, Department of Engineering Mechanics, Faculty of Vehicle Engineering and Mechanics, Dalian University of Technology, Dalian 116024, PR China

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Abstract

The paper presents a nonlinear Finite Element (FE) algorithm to simulate the inhomogeneous steady swelling of polymeric gels. The algorithm is developed based on the multiplicative decomposition of the deformation gradient into an elastic part and a swelling part. The corresponding constitutive framework and linearization of the FE equation are elaborated, which leads to an equivalent body force driving the materials to swell. A staggered iterative procedure is designed to ensure the strongly coupled chemical and mechanical fields to reach the equilibrium state simultaneously. The constitutive equations are constructed in the framework of the volumetric–isochoric splitting of the free energy function, which is helpful both for a different treatment of the incompressible part in the FE equation and for a physical interpretation of the coupling effects between the chemical and mechanical fields. In the present work, an additive free energy function, coupling the contributions of the Flory–Huggins model and the non-Gauss statistical–mechanical model, is adopted and the corresponding consistent tangent modulus in the current configuration is also derived. To implement the FE algorithm, two two-dimensional (2D) elements and one three-dimensional (3D) element are developed, which are validated by some analytical solutions, such as free swelling of gels in 2D and 3D cases, squeezing a swollen gel with uniform pressure and the constrained swelling of a single-layer and a core–shell gel ring. The algorithm is also proved to be capable of handling the surface instabilities and some engineering applications such as hydrogel-based composite beams and thin films.

Keywords: Polymeric gel; Swelling; Large deformation; Multiplicative decomposition; Staggered finite element algorithm

1. Introduction

A hydrogel is a cross-linked polymer network swollen by solvent molecules, which could give rise to a large morphological transformation after absorbing a large amount solution. These materials are playing an increasing important part in a diverse range of applications, such as drug delivery, tissue engineering, smart optical system and so on [1].

* Corresponding author.
E-mail addresses: liu.yin@mail.dlut.edu.cn (Y. Liu), zhanghw@dlut.edu.cn (H. Zhang), zhengyg@dlut.edu.cn (Y. Zheng).
[1] Tel.: +86 411 84706249; fax: +86 411 84706249.

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Gel swelling is a coupled process which is related to both mechanical and chemical fields and could be responsive to many kinds of stimuli, such as PH, temperature, light, electric field, ionic strength and humidity. Until now, vast contributions on modeling gel swelling have been elaborated, which could be divided into two categories: the theory of mixtures and the continuum-based theory. A full review of the contributions in this field is beyond the scope of the current work. Here, we just take a brief review on the continuum-based theory and the corresponding numerical implementations in the recent ten years and the earlier works have been well summarized in the works by, e.g., Hong et al. [2,3], Duda et al. [4] and Deng and Pence [5].

Many recent works absorbed nutrients from the classical contributions of Gibbs [6], Biot [7] and Flory and Rehner [8], in which, the theory of large deformation of solids with a growing fluid, the motion of a fluid in a porous elastic solid and the free energy function of the swelling gels were investigated, respectively. Based on their works, Hong et al. formulated a theoretical framework coupling mass transport and large deformation in polymeric gels [2] and implemented their theory in the commercial FE package, Abaqus, for the inhomogeneous steady response of swelling gels [3]. Then, Zhang et al. [9] and Toh et al. [10] extended their methods to the coupled transient analysis of swelling gels. Afterward, their theory found applications in the spherical swollen hydrogel containing a hard core [11], buckling of polymeric membrane thin film gels [12] and sealing pressure and the sealing time of a swelling packer [13]. Their impressive works make the simulation of gel swelling take a large leap from the laboratory to the engineering practice. Following their line of thought, further attempts on refining the numerical model have also been made. For example, Kang and Huang [14] developed a general formulation coupling mechanical and chemical equilibrium conditions, which is capable to implement numerical simulation of hydrogels swelling under various constraints. Then, Li et al. [15] proposed a numerical framework based on the improved complex variable element-free Galerkin method for the inhomogeneous swelling of gels and Juha [16] addressed a total Lagrangian formulation for gel swelling with the Flory–Rehner free energy function and the corresponding consistent linearized tangent moduli was also derived.

More recently, several researchers proposed to model the gel swelling in the framework of the multiplicative decomposition of the deformation gradient into an elastic part and a swelling part. For example, Duda et al. [4] developed a general finite-strain theory for the mutual interaction of mechanics and chemistry for solids capable of absorbing fluid-like chemical species, which could consider more general classes of mechanochemical environments, such as the gels that are not immersed in a fluid bath. Then, Chester and Anand [17] formulated a continuum theory to describe the coupled effects of fluid permeation and mechanical deformation, in which the related kinematics and the constitutive law based on the multiplicative decomposition were elaborated. The numerical implementation of their theory based on Abaqus is capable of modeling finite deformation, fluid permeation and heat transfer for thermally responsive gels [18], which is a remarkable progress for the numerical modeling of gels.

Besides, many other continuum based works were also developed concentrating on some specific aspects of gel swelling. For example, Dolbow et al. presented a hybrid extended finite-element/level-set method for modeling chemical induced volume transition in stimulus-responsive hydrogels [19,20] and Doi [21] also proposed a dynamical model involving coupling between elastic deformation and solvent permeation with application to the volume transition of gels. Lucantonio et al. [22] developed a theory for modeling the swelling process from an initially swollen, stress-free and homogeneous configuration. In addition, Baek and Srinivasa [23] developed a theoretical framework for modeling the slow diffusion of a fluid into a swelling solid undergoing large deformation, and then their model was employed to treat both saturated and unsaturated gels in equilibrium and subject to loading at the gel interface [24], where no additional fluid is available for uptake into the gel system. Similar treatments on this kind of gels could be found in Deng and Pence [5].

Though remarkable progresses in developing theoretical and numerical models have been made, some problems with regard to the numerical modeling remain unresolved or have not been clearly clarified. (1) As mentioned earlier, several recent contributions on gel swelling are based on the multiplicative decomposition of the deformation gradient, which provides an intuitional framework to understand and to model the swelling phenomena and could be extended to the anisotropic swelling without too much hard work. However, to the author's knowledge, the FE implementation based on the multiplicative decomposition, such as the consistent tangent modulus and the linearization of the nonlinear FE equation, and its difference with the traditional geometrically-nonlinear problems seem not to be resolved. Figuring out these problems could help the researchers reuse the developed nonlinear FE program to model swelling of gels more efficiently. (2) The variables of the mechanical and the chemical fields interacting with each other are strongly coupled. How to design the finite element algorithm to make these two fields reach the equilibrium state simultaneously? (3) Swollen gel is intrinsically a kind of hyperelastic material and always shows incompressible