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Diffusion of a fluid through a spherical elastic solid undergoing large deformations

J.S. Soares *

Department of Mechanical Engineering, 3123 TAMU, Texas A&M University, College Station, TX 77845-3123, United States

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ABSTRACT

The diffusion of a fluid through a spherical elastic solid undergoing large deformation is described in this paper. The constitutive model used is the single-constituent model for diffusion of fluids in nonlinear elastic solids, originally presented by Baek and Srinivasa [S. Baek, A.R. Srinivasa, Int. J. Nonlinear Mech. 39 (2004) 201–218] and based on a variational method and on the assumption of continuity of chemical potential across the solid–fluid interface. The balance laws for a single continuum with mass diffusion are cast in spherical coordinates, and suitable boundary conditions are posed to describe the radial diffusion of fluid through an elastic spherical shell with finite thickness. Its inner surface is adjacent to a rigid wall, either impermeable or permeable, while the outside surface is in contact with the fluid that swells the solid, diffuses through it, and exerts a hydrostatic pressure on its surface.

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1. Introduction

The aim of the present work is to demonstrate and improve the feasibility of Baek and Srinivasa single-constituent model (cf. [2]) in the description of a liquid (such as toluene) diffusing slowly into an elastic solid (such as rubber) that swells upon absorbing the liquid.

Polymer-based systems have had an enormous impact on drug delivery therapies [9]. The techniques employed today differ in concept but all of them share one particular feature, the mechanism of diffusion of certain species, the drug, through a matrix, usually polymeric in nature. In one approach, the drug is physically entrapped in a solid polymer capsule that can be then injected or implanted in the body. Early forms of these systems involved non-degradable polymers in membrane-controlled diffusion such as silicone rubber, which could release low molecular weight drugs for extremely long times [6]. Alternatively, drugs were also physically embedded in polymers at concentrations high enough to create a series of interconnecting pores through which the drug could afterward slowly diffuse from a matrix system [18]. Subsequently, biodegradable systems were utilized, where the combination of diffusion through pores as well as polymeric matrix degradation allows controllable release rates [8].

There are three distinct approaches to model such a system. The usual approaches using Fick's law and Darcy's law are too simple: the solid is assumed to be static, rigid, unaffected by the penetrating fluid, and thus cannot account for the swelling. On the other hand, the development of mixture theory and its application to the diffusion of fluids through elastic solids is a landmark of modern continuum mechanics achieved by Truesdell [20]. Since then an extensive collection of solutions for particular boundary value problems were obtained ranging from problems with finite media by Rajagopal and co-workers (cf. [5,7,16]) to the extension of such ideas for the development of other theories such as mixture theory for membranes

* Tel.: +1 979 845 9226; fax: +1 979 845 4450.
E-mail address: joao@tamu.edu

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[17]. However, some difficulties usually arise in specifying appropriate boundary conditions [12]. Mixture theory requires an extra assumption to be made on the division of tractions or displacements through the constituents at the boundary, information that is usually not available. Nevertheless, the predictions of such models agree exceedingly well with the experiments, but it had been shown that the results are quite insensitive to the boundary conditions [11].

Baek and Srinivasa's single-constituent model is composed of a polymeric elastic network with interstitial fluid. The constitutive response of the material is based on a thermodynamic framework for dissipative systems and is obtained using a variational technique related to the assumption of maximum rate of dissipation (a technique extensively applied to other problems, cf. [4,13,15] and references therein) concomitantly with the derivation of constraint responses through a limiting process (cf. [14]). The model was published in 2004 [2], and it was extended in such a way that the electric effects of the diffusing species could also be taken into account in the diffusion mechanism [3]. The authors had also shown that the model yields the same governing equations as mixture theory would for a binary mixture of an elastic solid and a diffusing fluid when restricted to quasi-static diffusion.

Baek and Srinivasa tackled the problem of the boundary condition using the concept of chemical potential and the assumption of its continuity through the interface between the swollen solid and the surrounding fluid. Baek and Srinivasa model is physically sound and achieves experimental concordance – data obtained by Paul and Ebra Lima [10] for the steady-state diffusion of an ideal fluid in the direction normal to the surface of an isotropic nonlinear elastic layer was well approximated with this approach when compared with its mixture theory counterpart. As opposed to boundary value problem describing the diffusion through an infinite slab published by Baek and Srinivasa [2], the problem presented in the present paper consists of a nonlinear elastic hollow solid sphere of finite thickness undergoing large deformations conjointly with steady-state radial diffusion of a fluid species through it. However, variational approaches may lead to difficulties when a fully dynamical problem is involved. Even within the context of purely elastic materials, one runs into difficulties.

Other physical meaningful cases yielding different boundary value problems were solved. In all of them, the outer surface of the spherical membrane was assumed to be traction-free and in contact solely with the surrounding fluid (i.e. the only traction imposed on this boundary is the radial fluid pressure), whereas in the interior interface, two different cases were considered: (1) a constrained displacement over a rigid impermeable wall where the equilibrium condition corresponds to the situation where no transmural flux occurs and is characterized by free swelling and a saturated solid and (2) constrained displacement over a rigid permeable wall where a flux is developed due to the pressure differential between outer and inner spaces (a similar BVP as the infinite slab considered in [2], but with a spherical layer).

The arrangement of this paper is as follows. In Section 2, the notation and kinematic quantities are defined, the equations of conservation of mass of the swollen solid and the fluid are presented, and the volume additivity constraint is introduced. In Section 3, general governing equations for mass diffusion trough the swollen solid derived by Baek and Srinivasa [2] are recorded. Section 4 particularizes the Helmholtz free energy function for elastic rubbers based on arguments drawn from statistical mechanics. Section 5 contains the application of the model for spherical coordinates and in Section 6 the boundary conditions for two boundary value problems considered are specified. Lastly, the numerical results obtained as the solution of the governing equations are presented and discussed in Section 7.

2. Preliminaries

Let us consider a body composed of a polymeric network which is homogeneous and incompressible in the dry state. This polymer is immersed in a fluid bath. Then, the polymer absorbs the surrounding fluid and it gradually swells. We shall henceforth call the mixture of polymer backbone chains and interstitial fluid molecules as the *swollen polymer*. Although the natural modeling approach for such class of problems would be to treat such material as a binary mixture within the context of mixture theory, Baek and Srinivasa [2] presented a single-constituent continuum approach which results in a simple set of equations. Furthermore, that they also had shown that the equations obtained with the single-constitutent approach are the same as the ones arising from mixture theory when the inertia effects are ignored.

Let the initial dry polymer and the swollen polymer at time t occupy configurations κ_0 and κ_t, respectively. As shown in Fig. 1, a closed system consists of a swollen polymer and surrounding fluid occupying the regions Ω_p and Ω_f, respectively. The fluid–solid interface and the system boundary are Γ_p and Γ_f, respectively, and their corresponding outward unit normals are $\mathbf{n}_1$ and $\mathbf{n}_2$.

The motion of the swollen polymer relatively to a reference configuration κ_0, the displacement, and the deformation gradient are given, respectively, by

$$\mathbf{x} = \boldsymbol{\chi}_{\kappa_0}(\mathbf{X}, t) \tag{1}$$

$$\mathbf{u} = \mathbf{x} - \mathbf{X} \tag{2}$$

$$\mathbf{F} = \frac{\partial \boldsymbol{\chi}_{\kappa_0}}{\partial \mathbf{X}} \tag{3}$$

where $\mathbf{X}$ and $\mathbf{x}$ are the positions of a polymer particle in κ_0 and κ_t, respectively.

The velocity of particles composing the swollen polymer is given by

$$\mathbf{v} = \left.\frac{\partial \boldsymbol{\chi}_{\kappa_0}}{\partial t}\right|_{\mathbf{X}\,\mathrm{fixed}} \tag{4}$$

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