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Diffusion and swelling in a bio-elastic cylinder

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Abstract

An analysis is presented of the equilibrium response of a radially deformed cylinder of isotropic, incompressible bio-elastic material swollen by an infused liquid satisfying a static diffusive balance law.

Keywords

Bio-elasticity; swelling; diffusion

1. Introduction

The inspiration for this work draws from the need for a predictive model of the mechanical response of biological tissue infused with a liquid. Among the many potential applications to biomechanics, we mention the elucidation of the role of fluid and nutrient transport in the process of growth and remodelling, and the effect of blood perfusion on the mechanical response of heart tissue. Quantitative analysis of these phenomena requires a modeling framework in which the coupled interplay between deformation and swelling, and the diffusion of fluid within the tissue [1-4], can be understood. To this end, we base the present analysis on the model of diffusion and swelling in finitely deforming elastomers developed in [4], adapted to the bio-elastic strain-energy function proposed in [5].

Our view is that the solution of certain simple problems characterized by relatively simple geometries and a high degree of symmetry offers considerable insight into the behavior of such models while avoiding the complexities associated with the development of sophisticated numerical methods required for general applications. Indeed, this philosophy underlies most of the history of modern finite elasticity theory and has given rise to a large number of important solutions which, in turn, have guided empirical work required to support the theory. This philosophy carries over to recent efforts to quantify the effects of swelling in elastomers [6-8], which are closely related to the present work. Thus, toward this aim, in the present, preliminary, work we confine attention to the axisymmetric response of a

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cylinder undergoing plane-strain radial deformation in the presence of a two-dimensional radial distribution of diffusant concentration. The deformation and concentration are controlled by differential equations expressing mechanical equilibrium and the balance of diffusive flux.

The basic theory for two-dimensional response is recalled in Section 2 and its specialization to isotropic bio-elastic materials is outlined in Section 3. In Section 4 we present the further specialization of the theory to axisymmetric radial deformations and we conclude, in Section 5, with a discussion of associated numerical solutions.

2. Basic theory

We base our analysis on a simple model of diffusion in nonlinearly elastic materials developed in [4]. In view of our *a priori* restriction to plane-strain deformations, we confine attention to the purely two-dimensional formulation discussed in Section 3 of that work. The remainder of this section is devoted to a brief outline of the relevant theory. Interested readers are encouraged to consult [4] for a fuller exposition.

Let $\Psi(\mathbf{F}, c)$ be the strain energy of a uniform material, per unit area of a fixed reference configuration, where $\mathbf{F}$ is the gradient of the deformation $\mathbf{y} = \chi(\mathbf{x})$ and c is the concentration of diffusant. The reference configuration is identified with the initial configuration of the dry elastomer and $\mathbf{x}$ is the position of a material point of the dry elastomer in this configuration. The deformation gradient and concentration satisfy the *swelling constraint*

$$J = 1 + c, \quad (1)$$

appropriate for an incompressible elastomer infused with an incompressible liquid. Here $J = \det \mathbf{F}$ and c is the area of diffusant present in the gel per unit area of dry elastomer.

The Piola stress, $\mathbf{P}$, is given by

$$\mathbf{P} = \Psi_{\mathrm{F}} - q\mathbf{F}^{*}, \quad (2)$$

where $\Psi_{\mathbf{F}}$ is the derivative of Ψ with respect to $\mathbf{F}$ at fixed c, $\mathbf{F}^*$ is the cofactor of $\mathbf{F}$ and q is a Lagrange multiplier associated with the swelling constraint. The latter also figures in the expression

$$\mu = q + \Psi_{c} \quad (3)$$

for the *chemical potential* μ, where Ψ_c is the derivative with respect to c at fixed $\mathbf{F}$.

Here and henceforth we assume that sufficient liquid is available to support unlimited uptake by the gel. The alternative, corresponding to an unsaturated condition [9, 10], entails the constraint that the total dilation reduce to the sum of the elastomer and liquid areas. This

constraint is global in nature and carries a uniform Lagrange multiplier, in contrast to the local multiplier q of the present model.

Let **m** be the diffusive flux vector. This satisfies the dissipation inequality [4]

$$\mathbf{m} \,.\, \nabla\mu \leq 0 \quad (4)$$

and figures in the diffusive balance

$$\dot{c} + div\mathbf{m} = 0, \quad (5)$$

where the dot refers to the time derivative at fixed reference position **x**. Here *div* is the referential two-dimensional divergence based on **x**.

Following standard practice, we view the dissipation inequality as a restriction on the constitutive equation for the diffusive flux. For example, if the flux depends on the list $\{\mathbf{F}, c, \nabla\mu\}$, then an important theorem due to Gurtin (see [11]; Chapter 9, Section b.2) implies that the dissipation inequality yields the existence of a tensor function $\mathbf{M}(\mathbf{F}, c, \nabla\mu)$ - the *mobility tensor*- such that

$$\mathbf{m} = \mathbf{M}(\mathbf{F}, c, \nabla\mu)\nabla\mu, \quad (6)$$

with $\nabla\mu \cdot \mathbf{M}\nabla\mu \leq 0$. In the important special case in which **M** is independent of $\nabla\mu$, this requires that **M** be negative semi-definite.

The balance laws consist of (5) and

$$div\mathbf{P} = 0, \quad (7)$$

corresponding to mechanical equilibrium without body force. Chemical equilibrium is associated with the restriction

$$\mu = 0 \quad (8)$$

which implies the vanishing of the diffusive flux and hence the cessation of evolution of the concentration. Of course a static concentration field is always achieved provided that

$$div(\mathbf{M}\nabla\mu) = 0\,. \quad (9)$$

The system of equations to be solved in this work consists of the swelling constraint (1), the force balance (7) and the static diffusive balance (9), augmented by suitable boundary

conditions. Typical boundary conditions entail the specification of μ or $\mathbf{m}\cdot\nu$ on complementary parts of the boundary, with exterior unit normal ν, and position $\mathbf{y}$ or traction

$$\mathbf{p}=\mathbf{P}\mathscr{V} \quad (10)$$

on (possibly different) complementary parts. In this work we impose pressure boundary conditions for which

$$\mathbf{p}=-p^{\mathbf{F}^*}\mathscr{V}, \quad (11)$$

where p is the pressure intensity.

3. Swelling in isotropic materials

We assume the gel to be isotropic. Concerning its constitutive response, we adopt the widespread assumption that stress is generated by elastic deformation $\mathbf{H}=\mathbf{F}\mathbf{G}^{-1}$ measured from a stress-free swollen state, where

$$\mathbf{G}=(1+c)^{1/2}\mathbf{I}, \quad (12)$$

is the swelling deformation and $\mathbf{I}$ is the two-dimensional identity. From (1), we conclude that $\det\mathbf{H}=1$, which comports with the assumed incompressibility of the solid component of the gel.

The strain energy W, per unit area of the *swollen* state, is defined by $\Psi=(\det\mathbf{G})W$ and we assume that it depends on the deformation via $\mathbf{H}$; thus,

$$\Psi=(1+c)W(\mathbf{H},c), \quad (13)$$

in which the explicit dependence of W on c is intended to model chemical interaction between the solid component of the gel and the diffusant. In the polymer literature it is conventional to adopt Flory's formulation of this interaction. However, this is known to be inappropriate for biological tissues [12]. In any case, we are concerned in the present work with the effects of a purely mechanical swelling interaction and thus assume that W is determined by $\mathbf{H}$ alone. Accordingly,

$$\Psi(\mathbf{F},c)=(1+c)W((1+c)^{-1/2}\mathbf{F}). \quad (14)$$

We adopt the strain-energy function for incompressible isotropic materials due to Demiray [5] for the elastic response of biological tissues in the absence of swelling. For three-dimensional deformations in the case of pure elasticity ($c=0$), this is given by

$$W(\mathbf{F}) = (G / 2\gamma)\{\exp[\gamma(tr\mathbf{C} - 3)] - 1\}, \quad (15)$$

where $\mathbf{C} = \mathbf{F}^t\mathbf{F}$ is the right Cauchy-Green deformation tensor, G is the ground-state shear modulus and γ is a dimensionless parameter. For isochoric plane-strain deformations it is easily demonstrated that

$$tr\mathbf{C} = I^2 - 1, \quad \text{where} \quad I = tr\mathbf{U} \quad (16)$$

and $\mathbf{U}$ is the *two-dimensional* right-stretch tensor. Accordingly, the plane-strain energy is

$$W = (G / 2\gamma)\{\exp[\gamma(I^2 - 4)] - 1\}, \quad (17)$$

in which G now has dimensions of force/length.

To adapt this energy to two-dimensional swelling, we use (17) with $W(\mathbf{H}) = w(H)$, where

$$w(H) = (G / 2\gamma)\{\exp[\gamma(H^2 - 4)] - 1\}, \quad (18)$$

and H is the trace of the right-stretch factor in the polar decomposition of $\mathbf{H}$. From (12), this is given simply by

$$H = I / \sqrt{1 + c}\,. \quad (19)$$

Accordingly, $\Psi(\mathbf{F}, c) = \psi(I, c)$, where

$$\psi(I, c) = (G / 2\gamma)(1 + c)\{\exp[\gamma(I^2 / (1 + c) - 4)] - 1\}, \quad (20)$$

and the stress is [4]

$$\mathbf{P} = \Psi_I\mathbf{R} - q\mathbf{F}^*, \quad (21)$$

where $\mathbf{R}$ is the rotation in the polar factorization of $\mathbf{F}$.

Concerning the mobility tensor, the most general two-dimensional form compatible with isotropy is [4]

$$\mathbf{M} = \beta_0\mathbf{I} + \beta_1\mathbf{U} \quad (22)$$

in which $\beta_{0,1}$ are functions of I and c. However, due to the paucity of empirical information about these functions, we adopt the classical form

$$\mathbf{M} = D\mathbf{I} \quad (23)$$

in which D, the diffusivity, is a negative constant; then, (9) reduces to Laplace's equation

$$div(\nabla \mu) = 0, \quad (24)$$

where

$$\mu = q + \psi_c . \quad (25)$$

4. Axisymmetric response of a cylinder

We consider a purely radial deformation

$$\chi(\mathbf{x}) = \lambda(R)\mathbf{x} \quad \text{with} \quad \lambda(R) = r(R) / R \quad \text{and} \quad R = |\mathbf{x}|, \quad (26)$$

where r is the radius of the circle $R = const.$ after deformation. The deformation gradient is

$$\mathbf{F} = \lambda\mathbf{I} + R^{-1}\lambda'(R)\mathbf{x} \otimes \mathbf{x}, \quad (27)$$

which may be recast as

$$\mathbf{F} = r'(R)\mathbf{u} \otimes \mathbf{u} + (r / R)\mathbf{v} \otimes \mathbf{v}, \quad (28)$$

with $\mathbf{u} = \mathbf{x}/R$ and $\mathbf{v} = \mathbf{k} \times \mathbf{u}$, where $\mathbf{k}$ is a unit normal to the plane of deformation. This yields

$$\mathbf{F}^* = (r / R)\mathbf{u} \otimes \mathbf{u} + r'(R)\mathbf{v} \otimes \mathbf{v} \quad (29)$$

and

$$J = (r / R)r', \quad (30)$$

and hence the requirement that $r' > 0$. Accordingly, $\mathbf{R} = \mathbf{I}$, $\mathbf{U} = \mathbf{F}$ and

$$I = R^{-1}(Rr)' . \quad (31)$$

Invoking the Piola identity $div\mathbf{F}^* = \mathbf{0}$, the equilibrium equation (7) may be reduced to

$$\nabla(\psi_I) = \mathbf{F}^* \nabla_q . \quad (32)$$

The swelling constraint, combined with (30), implies that the concentration c is a function of R alone. Then, for uniform materials, $\nabla(\psi_I) = (\psi_I)' \mathbf{u}$. With (29), we conclude that q depends on R alone, and is such that

$$(\psi_I)' = (r / R) q' . \quad (33)$$

Equation (25) implies that μ is also a function of R, so that (24) reduces to

$$R^{-1}(R\mu')' = 0 . \quad (34)$$

The formulation is completed by appending boundary conditions. Concerning these, we assign a value μ_A of the chemical potential at the inner radius $R = A$, and the diffusive flux at the outer radius $R = B$. With $\nu = \mathbf{u}$ at the outer boundary, we thus assign a value $\mathbf{m} \cdot \mathbf{u} = M$ there; then, $D\mu' = M$ at $R = B$. An *in*flux of diffusant corresponds to $M < 0$. Because $D < 0$, the ratio M/D is then positive, and the function $\mu(R)$ is easily found to be

$$\mu(R) = \mu_A + (M / D) B \ln(R / A), \quad (35)$$

which couples the deformation to the Lagrange multiplier q via (25). Chemical equilibrium is recovered by setting μ_A and the flux M to zero.

Finally, we assign a pressure p at the inner radius and zero pressure at the outer radius. Using (11), (21) and (29), these are found to correspond to the boundary conditions

$$\psi_I - q(a / A) = -p(a / A) \quad \text{at} \quad R = A \quad (36)$$

$$\psi_I - q(b / B) = 0 \quad \text{at} \quad R = B \quad (37)$$

where $a = \imath(A)$ and $b = \imath(B)$.

The swelling constraint (1) and the equilibrium equation (33) furnish a differential-algebraic system of two equations for the concentration field $c(R)$ and the deformation $\imath(R)$.

5. Simulations

Numerical solutions to the foregoing system are obtained using a shooting method based on a Runge-Kutta integration scheme. Length is non-dimensionalized by the inner reference radius A and all simulations pertain to annular region defined by $1 \leq R/A \leq 1.25$ with $\gamma = 0.03$ in (20) [5].

In the solution procedure we combine (20), (25) and (35) to evaluate the Lagrange multiplier q in terms of the deformation and concentration fields. Fixing a value of b/B, where $B/A = 1.25$, we solve (37) for the value of the concentration c at the outer radius. Equation (33) is then backward integrated from $R/A = 1.25$ to obtain the deformation r/A and hence the value of a/A at $R/A = 1$, and finally (36) is used to compute the corresponding inflation pressure at the inner boundary. In this way values of a/A may be correlated with values of the pressure.

The case of purely elastic response, corresponding to $c = 0$, is treated differently. The deformation is then given simply by

$$(r / A)^2 - (a / A)^2 = (R / A)^2 - 1, \quad (38)$$

and (38) is used with a fixed value of b/B to compute the boundary value of the Lagrange multiplier for use in a backward integration scheme to determine the field q from (33). Evaluating (38) at $R = B$, the value of a/A is obtained and used in (36) to compute the inflation pressure. The response is depicted in Fig. 1 in terms of the relation between pressure and dimensionless wall thickness, h/H, where $h = b - a$ and $H = B - A$, together with the pressure-enclosed area relation. Variations of the hoop and radial principal stretches, r/R and $r'(R)$ respectively, and the Lagrange multiplier q, in the interior of the cylinder are also shown. We draw particular attention to the expected prediction of thinning of the cylinder under inflation.

The interplay between diffusion and deformation is illustrated in Fig. 2, for a particular value of the chemical potential at the inner boundary and diffusive flux $M^* = (MB)/(DG)$ at the outer boundary. This generates a concentration field in the interior that varies with inflation pressure, which in turn modifies the distributions of the principal stretches and the Lagrange multiplier accordingly. A significant departure of the relation between pressure and wall thickness relative to the case of pure elasticity is evident. This is due to swelling of the material, yielding a counter-intuitive thickening of the cylinder upon inflation. In this and subsequent figures the concentration and Lagrange multiplier fields are plotted against deformed radius to better highlight the effect of varying the inflation pressure.

Figure 3 depicts the effect of varying the assigned flux at zero inflation pressure with $\mu_A = 0$. As expected, higher levels of flux promote increased levels of swelling in the material and correlate with higher levels of wall thickness. A significant effect on the interior stretch distributions is also predicted.

Finally, Fig. 4 illustrates the response under conditions of chemical equilibrium, corresponding to vanishing chemical potential throughout the cylinder (i.e., μ_A and M vanish

in (35)). This corresponds to contact of the cylinder with a liquid bath at zero chemical potential at its inner and outer radii. In this case the distributions of the stretches, the concentration and the Lagrange multiplier are predicted to be nearly uniform throughout the cylinder. Further, the value of concentration required to maintain chemical equilibrium increases with inflation pressure, giving rise once again to thickening of the cylinder upon inflation.

Our simple model predicts a dramatic effect of diffusion and swelling on the mechanical response of biological tissues under a variety of conditions. Accordingly, it is expected that coupling between deformation and diffusion will play a significant role in the development of more general predictive models for application to biomechanics.

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Highlights

- The interplay between deformation and liquid-induced swelling in biological tissues is modelled in the setting of a simple axisymmetric boundary-value problem. The model accounts for liquid diffusion in the tissueand accommodates general boundary conditions. The study demonstrates that diffusion and swelling have a dramatic effect on mechanical response.

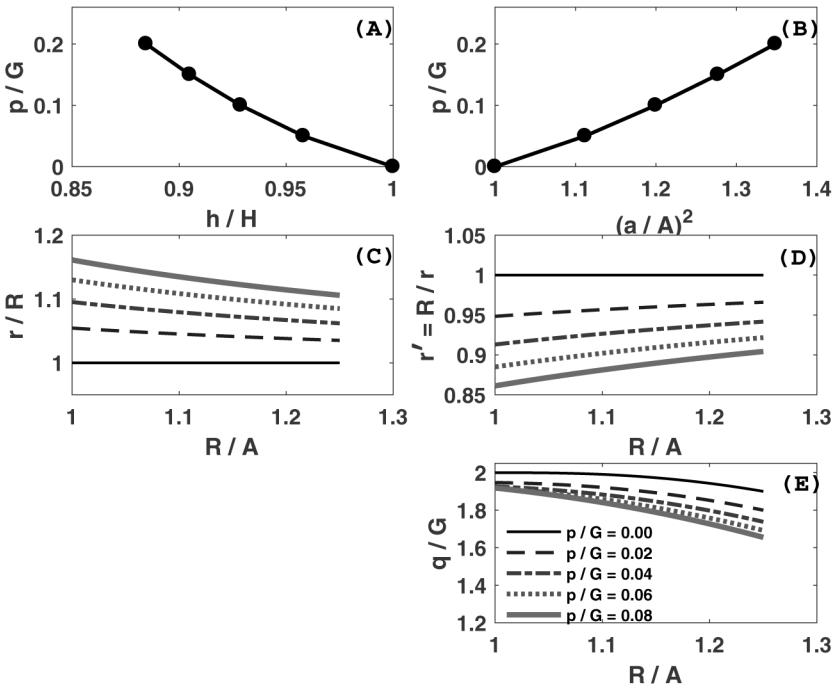

Figure 1:

Purely mechanical response. (A) Inflation pressure versus deformed wall thickness, (B) Inflation pressure versus deformed cavity area, (C) Hoop stretch as a function of reference radius, (D) Radial stretch as a function of reference radius, (E) Lagrange multiplier as a function of reference radius. Note: the legends in panels (C) and (D) are shown in panel (E).

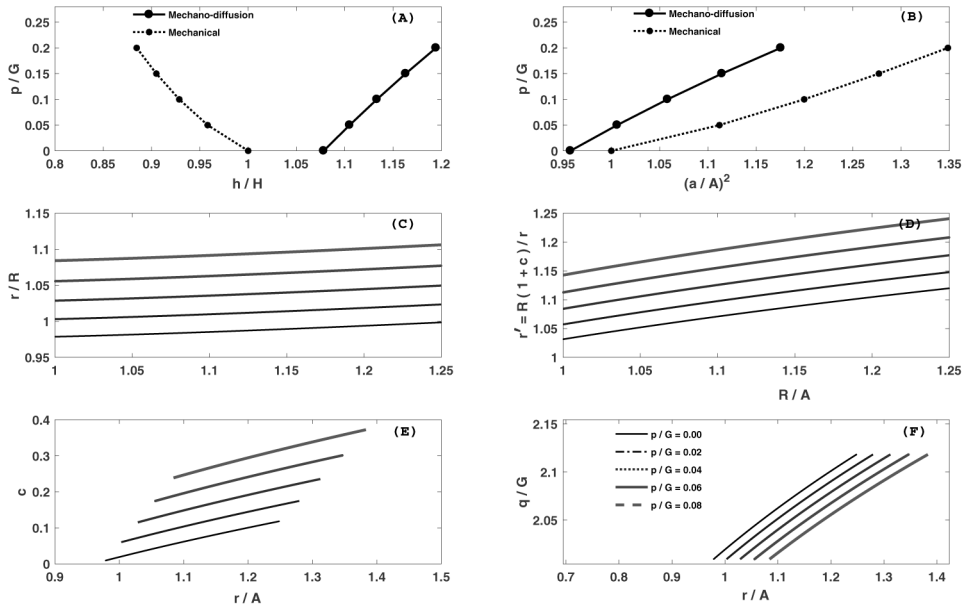

Figure 2:

Coupled mechano-diffusion. (A) Inflation pressure versus deformed wall thickness, (B) Inflation pressure versus deformed cavity area, (C) Hoop stretch as a function of reference radius, (D) Radial stretch as a function of reference radius, (E) Diffusant concentration as a function of deformed radius, (F) Lagrange multiplier as a function of reference radius. Note: the legends in panels (C), (D), and (E) are shown in panel (F).

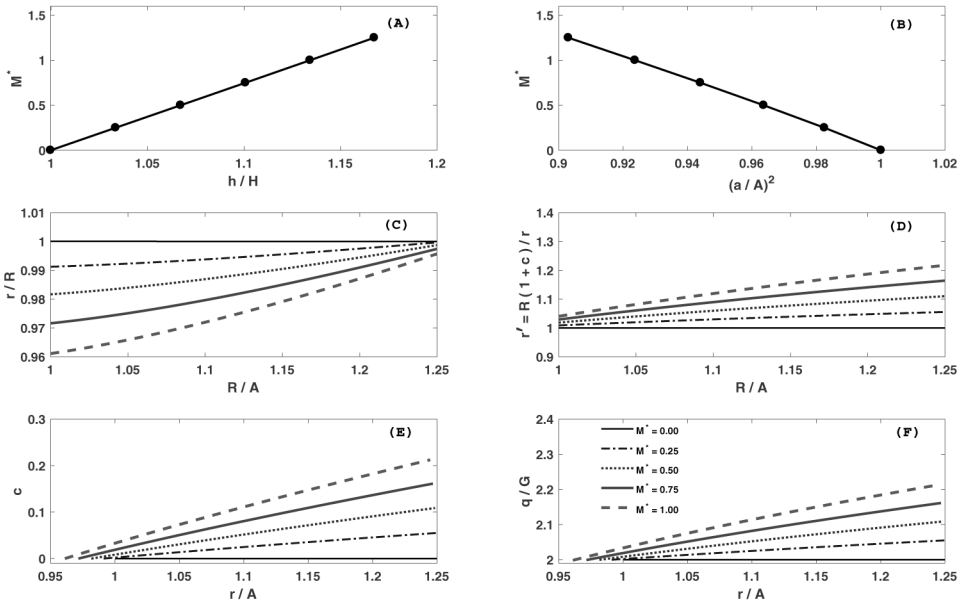

Figure 3:

Coupled mechano-diffusion. (A) Assigned flux versus deformed wall thickness, (B) Assigned flux versus deformed cavity area, (C) Hoop stretch as a function of reference radius, (D) Radial stretch as a function of reference radius, (E) Diffusant concentration as a function of deformed radius, (F) Lagrange multiplier as a function of reference radius. Note: the legends in panels (C), (D), and (E) are shown in panel (F).

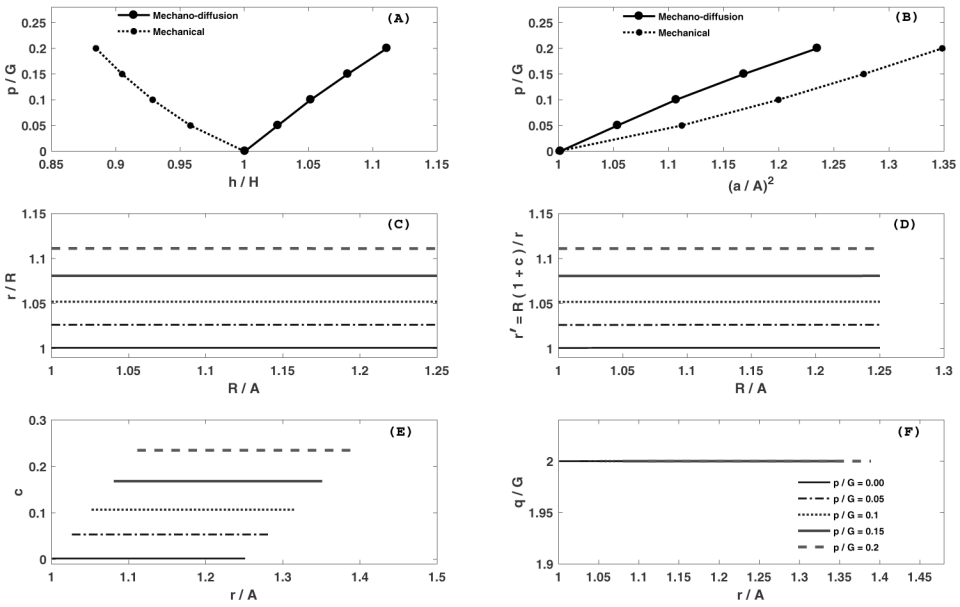

Figure 4:

Response at chemical equilibrium. (A) Inflation pressure versus deformed wall thickness, (B) Inflation pressure versus deformed cavity area,, (C) Hoop stretch as a function of reference radius, (D) Radial stretch as a function of reference radius, (E) Diffusant concentration as a function of deformed radius, (F) Lagrange multiplier as a function of reference radius. Note: the legends in panels (C), (D), and (E) are shown in panel (F).