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Strain assisted diffusion: Modeling and simulation of deformation-dependent diffusion in composite media

D. Klepach [b,*], T.I. Zohdi [a]

[a] Department of Mechanical Engineering, University of California, 6195 Etcheverry Hall, Berkeley, CA 94720-1740, USA
[b] Department of Mechanical Engineering, University of California, 6102 Etcheverry Hall, Berkeley, CA, USA

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ABSTRACT

In this work, we develop a model for strongly-coupled, deformation-dependent diffusion in composite media at finite strains. The coupling incorporates the effects of deformation into the diffusivity tensor. A time-transient, three-dimensional variational formulation is developed and then discretized using the Finite Element Method in conjunction with an implicit staggering scheme to resolve the coupled multiphysics. Numerical examples are provided to illustrate the model.

1. Introduction

In many modern engineering applications, diffusion in solids plays a major role in the operation of devices which are, in many cases, constructed from composite media. As a species diffuses into a solid, a complex physical process occurs, which primarily manifests itself as macroscopic swelling. The diffusion process can have a major effect on the operation resulting in large deformations and stresses and, in some cases, failure. In this paper, we investigate the phenomena of strong coupling between diffusion of a species into a nonlinear elastic solid body and the concentration, deformation, and stresses in that body. We are particularly interested in fiber-reinforced composite materials with different mechanical and diffusive properties. We consider cases where the diffusion and deformation are coupled in both directions, i.e. they affect one another. We first investigate the qualitative behavior analytically, then the time-transient, three-dimensional behavior for composite systems by developing a variational formulation which is then discretized using the Finite Element Method, in conjunction with an implicit staggering scheme.

Specifically, in this study we construct mathematical models where we begin with the separate, well-established, models for diffusion and finite elasticity. For diffusion, we consider enhancements to Fick's laws of diffusion. For elasticity, we consider a moderate finite strain elastic model employing a Kirchhoff–Saint Venant material. We consider material constants to be coupled and consider strain-dependent diffusivity, where the diffusivity tensor depends on the volumetric strain through the Jacobian $J = det(\boldsymbol{F})$. We also consider saturation effects, where a finite amount of diffusing species is absorbed by the solid and the diffusion process terminates. This is modeled as having a diffusivity tensor that is dependent on species concentration.[1] Early work on the coupling of diffusion and deformation or stress was done by Truesdell [1] Green and Adkins [2], and Adkins [3,4] have made major advancements in the field. Later on, Aifantis et al. [5–7] did work on stress-assisted diffusion, and also *Mixture theory* was used to model the coupling by Rajagopal [8]. In the last decade or so, there were recent theoretical advancements in nonlinear diffusion and mechanics that we found to be most relevant to this study. Baek and Srinivasa [9] came up with a more direct approach that deals with the problem and compared it with mixture theory, finding both theories to be comparable. Suo et al. analyzed large deformations in gels [10], which was useful in the development of the present model. For more complex modeling, including damage and thermal effects, see Zohdi [11] and Duda et al. [12].

2. Modeling deformation-dependent diffusion

We establish the basic settings of this model in the reference configuration. Capital letters are associated with the reference configuration and lower-case letters are associated with the current configuration. Letters with a tilde $(\tilde{\square})$ are associated with diffusive

* Corresponding author. Tel.: +1 972538237381.
E-mail address: klepachd@berkeley.edu (D. Klepach).

[1] For example, one could describe this by specifying that above a certain level of concentration the values of diffusivity tensor would drop to zero.

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processes, and the letters without any sign are mechanical variables. For three dimensional diffusion, the most common constitutive laws are known as Fick's laws, where the flux is related to the gradient of the concentration of a substance, $\widetilde{C}$, at a material point as,

$$\widetilde{\mathbf{J}} = -\widetilde{\mathbf{D}}Grad(\widetilde{C}). \tag{1}$$

where $\widetilde{\mathbf{D}}$ is the diffusivity tensor. Conservation of mass in a material point with no internal source terms can be written,

$$\frac{\partial \widetilde{C}}{\partial t} = -Div(\widetilde{\mathbf{J}}), \tag{2}$$

where *Div* is the divergence operator with respect to the reference configuration. Combining the two Eqs. (1), (2) yields

$$\frac{\partial \widetilde{C}}{\partial t} = Div(\widetilde{\mathbf{D}}Grad(\widetilde{C})) \tag{3}$$

which is known as Fick's law of diffusion. For mechanics, we use the balance of linear momentum

$$Div(\mathbf{P}) + \rho_{ref}\mathbf{f}_{ref} = \rho_{ref}\ddot{\mathbf{u}}_{ref} \tag{4}$$

where $\mathbf{P}$ is the first Piola–Kirchhoff stress, $()_{ref}$ implies the reference configuration, ρ is the mass density,$\mathbf{f}$ are the body forces, and $\ddot{\mathbf{u}}_{ref}$ is the second time derivative of the displacement. For elasticity, we consider a Kirchhoff–Saint Venant nonlinear elastic material model

$$\mathbf{S} = \mathbb{E} : \mathbf{E} \tag{5}$$

where $\mathbf{S}$ is the Second Piola–Kirchhoff stress and $\mathbf{E} = \frac{1}{2}(\mathbf{C} - \mathbf{I})$ is the Green–Lagrange strain tensor. We define the strains due to diffusion as $\mathbf{E}_c$, and consider the diffusion tensor, $\widetilde{\mathbf{D}}$, to be a function of the mechanical deformation and the concentration as,

$$\widetilde{\mathbf{D}} = \widetilde{\mathbf{D}}(\mathbf{E}, \widetilde{C}). \tag{6}$$

This allows us to construct mathematical models which describe different physical phenomena. The modified Second Piola–Kirchhoff stress becomes

$$\mathbf{S} = \mathbb{E} : (\mathbf{E} - \mathbf{E}_c) \tag{7}$$

and the modified diffusion equation becomes

$$\frac{\partial \widetilde{C}}{\partial t} = Div(\widetilde{\mathbf{D}}(\mathbf{E}, \widetilde{C})Grad(\widetilde{C})) \tag{8}$$

where *Grad* is the gradient operator with respect to the reference configuration.

3. Strain-dependent diffusivity

We assume that the diffusivity tensor, $\widetilde{\mathbf{D}}$, is a function of the deformation in general, and specifically a function of the volume change through the Jacobian as

$$\widetilde{\mathbf{D}} = \widetilde{\mathbf{D}}(J). \tag{9}$$

Some simple arguements provide guidance on constructing a model for $\widetilde{\mathbf{D}}(J)$. For example, if we continuously compress the material, it is reasonable to assume that the diffusivity will decrease to a lower limit (becoming fully densified), which we will take to be equivalent to zero diffusivity. As the volume increases, the magnitude of the diffusivity will grow to values larger than of the reference configuration ($J > 1$). In terms of a function, we require that $\widetilde{\mathbf{D}}(J = 0) = \mathbf{0}$, $\widetilde{\mathbf{D}}(J = 1) = \widetilde{\mathbf{D}}_0$. The actual values are material dependent, and can be found experimentally. We also assume that the function is smooth and continuous. A function that satisfies these requirements is the following:

$$\widetilde{\mathbf{D}}(J) = \widetilde{\mathbf{D}}_0 \frac{e^{aJ} - 1}{e^a - 1} \tag{10}$$

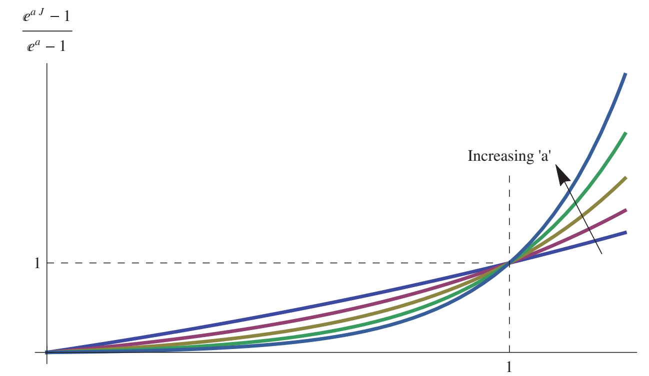

Fig. 1. Volume dependent diffusivity.

where 'a' is a constant that is determined experimentally. For the case where there are no deformations, the diffusivity tensor scales to its initial value $\widetilde{\mathbf{D}}_0$. The plot for Eq. (10) can be seen in Fig. 1.

4. Swelling strains

We now consider some simple models for swelling strains (i.e. $J > 1$).

4.1. Uniform swelling

In the simplest case, similar to thermo-elasticity, we consider uniform (isotropic, or direction-independent swelling, i.e. see [11]) defined via

$$\mathbf{E}_C = \beta(\widetilde{C} - \widetilde{C}_0)\mathbf{I} \tag{11}$$

where $\widetilde{C}_0$ is a material initial concentration and β is a scalr material constant that controls the magnitude of the stress resulting from the swelling (similar to the coefficient of volumetric thermal expansion, α_K, in thermo-elasticity). This yields the Second Piola–Kirchoff stress as

$$\mathbf{S} = \mathbb{E} : (\mathbf{E} - \beta(\widetilde{C} - \widetilde{C}_0)\mathbf{I}). \tag{12}$$

4.2. Non-uniform swelling

Alternatively, one may assume that the solid swells up non-uniformly (i.e anisotropic, or directionally-dependent). Specifically, it has preferred directions in which it will swell (i.e. along the direction of material fibers). We define β as a material constant, and $\mathbf{M}$ is a unit vector normal to the plane of isotropy in the reference configuration (i.e. $\mathbf{M}$ is in the direction of the fibers in a fiber-composite material). We assume that the material will swell up in any direction normal to the fiber direction, thus we use the projection tensor $\mathbf{I} - \mathbf{M} \otimes \mathbf{M}$. With that, we define the stress as,

$$\mathbf{S} = \mathbb{E} : [\mathbf{E} - \beta(\widetilde{C} - \widetilde{C}_0)(\mathbf{I} - \mathbf{M} \otimes \mathbf{M})] \tag{13}$$

Remark. As mentioned earlier, beyond a certain concentration level $\widetilde{C}_1$ (which is a material constant), the diffusivity is set to zero so that the diffusion process is terminated. Below a certain concentration level $\widetilde{C}_0$ (again, a material constant) it should initially retain its initial value of $\widetilde{D}_0$. In the range $[\widetilde{C}_0, \widetilde{C}_1]$ smoothly, we define the diffusivity as

$$\widetilde{D}(\widetilde{C}) = \widetilde{D}_0 - (\widetilde{D}_0 - \widetilde{D}_1) / \left(exp\left(\frac{\frac{\widetilde{C}_0 + \widetilde{C}_1}{2} - \widetilde{C}}{\alpha} \right) + 1 \right) \tag{14}$$