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A three-field (displacement–pressure–concentration) formulation for coupled transport–deformation problems

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ABSTRACT

This paper provides a three-field finite element formulation for the evaluation of coupled transport–deformation problems. A stabilized advection–diffusion–reaction model is employed to idealize the mass transport of an aggressive environmental agent within a solid medium, whereas the deformation response of the medium is formulated using the mixed finite element approach with pressure and displacement as unknown variables. The proposed model accurately captures the pressure and pressure gradient fields that characterize the reaction and advection terms of the mass transport model. The concentration-dependent viscoplastic deformation response is idealized using a generalized Johnson–Cook plasticity model. The accuracy characteristics of the proposed three-field formulation are assessed by numerical simulations, which indicate the significance of accurate estimation of pressure at high stress gradient zones for correct characterization of mass transport.

1. Introduction

Aggressive environmental elements deteriorate the mechanical performance of material and structural systems subjected to combined loading and environmental conditions. Examples of engineering problems that display environmental-deformation response coupling are manifold. Two problems that have received significant attention, among others, are hydrogen- and oxygen-induced embrittlement in metals [1,2].

Predictive computational modeling of the deformation response of such materials and structures subjected to aggressive environmental agents remains to be a significant challenge. The first difficulty is accurately modeling the coupling mechanisms between the inelastic deformation process and the mass transport of the aggressive agent into the structural material. The second difficulty is the development of a computational solution method to accurately evaluate the response in the presence of the coupling mechanisms. An extensive literature exists in characterization and modeling of metals subjected to hydrogen; and to a lesser extent, oxygen. The mass transport of the aggressive agent into the solid substrate is often modeled as a diffusion–advection–reaction problem [3], whereas the mechanical response involves inelastic deformations induced by the mechanical and thermal loads, as well as the environmental effects. Time-dependent deterioration of the mechanical properties is marked by the coupling between the transport process of the aggressive agent and the deformation under mechanical and thermal loads. The transport process typically results in volumetric expansion, hardening, embrittlement, loss of fatigue life and strength [4,5]. On the other hand, the chemical potential that drives the kinetics of the aggressive agent ingress is a function of the state of stress and deformation through formation of trap sites (e.g., dislocations) and microcracks that enhance the rate of mass transport.

Computational modeling of this phenomenon requires accurate capturing of the coupling effects between the transport and deformation mechanisms. Oskay and Haney [6] proposed a coupled transport–deformation formulation to simulate the oxygen-induced embrittlement of titanium structures. This formulation does not account for the advection–reaction terms that become significant at high stress gradient zones. The seminal work of Sofronis and McMeeking [3] provided the first finite element model for the coupled hydrogen transport - deformation response that can describe the hydrogen transport into a metal substrate around crack tips. This model has been extended to properly account for transport between trap and lattice sites by Krom et al. [7]. Ndong-Mefane et al. [8] addressed the potential instability problems in advection-dominated transport around crack and notch tips by employing a stabilized finite element approach. The advection coefficient, which depends on the pressure gradient, is typically approximated a posteriori through discrete differentiation of the pressure estimates at the integration points in a displacement-based finite element solution of the deformation problem. This leads to significant approximation errors at regions of high stress gradients such as notch and crack tips.

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In this paper, we propose a three-field computational model for the evaluation of coupled transport–deformation problems. The displacement, pressure and concentration fields are evaluated as independent unknowns. The key novel contribution of the present paper is the demonstration that the mixed finite element method, in which the pressure is treated as an independent unknown in addition to the displacement degrees of freedom, can be employed to accurately compute the pressure gradient in the deformation problem. The pressure gradient information, in turn, is employed to accurately calculate the instantaneous coefficients of the advection–reaction terms of the mass transport problem. In addition, the computational model has the following properties: (a) the mass transport problem is stabilized to accurately describe the advection-dominated transport in the presence of high stress gradients (e.g., crack and notch tips); (b) the deformation problem is evaluated using a tight-coupled two-field (displacement–pressure) formulation, whereas the transport and deformation processes are evaluated based on a staggered approach to efficiently address problems where the time scales associated with the transport and deformation processes are disparate.

The remainder of the paper is organized as follows: Section 2 provides the mass transport model with diffusion–advection–reaction terms coupled to a viscoplasticity model. In Section 3, the finite element model of the coupled physics problems based on the three-field (displacement–pressure–concentration) modeling is described, including the stabilization of the mass transport problem for advection-dominated problems. The details of the implementation of the proposed approach is included. Numerical verification studies to assess the performance of the model in the context of the oxygen ingress problem in titanium alloys are discussed in Section 4. Section 5 provides the conclusions and discussion of future research directions.

2. Problem statement

Consider the domain of an arbitrary solid body, $\Omega \subset \mathbb{R}^{n_{sd}}$, subjected to an aggressive agent along a part of the domain boundary, $\Gamma = \partial\Omega$, as illustrated in Fig. 1 (n_{sd} is the number of space dimensions). When subjected to elevated boundary concentration, fluxes applied on the domain boundary or stress gradient fields, the aggressive agent tends to diffuse into the body. Concurrently, the solid body is subjected to time varying mechanical loading. In this section, the governing equations of the aggressive agent transport and deformation processes are provided, and the coupling mechanisms between the two physical processes are described.

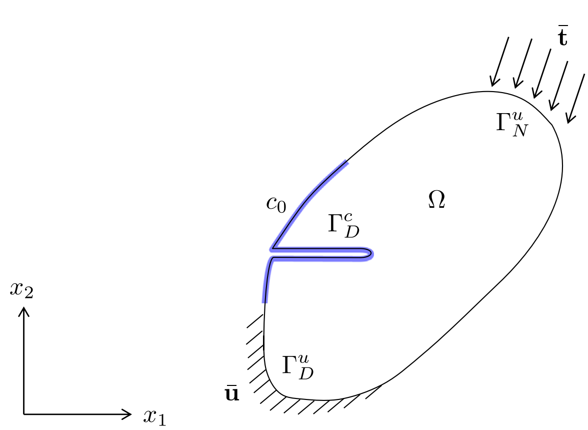

Fig. 1. Coupled transport–deformation processes defined on the problem domain, Ω.

2.1. Transport model

We adopt Oriani's equilibrium theory to describe the diffusion of the aggressive agent into the stressed solid [9]. According to this theory, the driving force for diffusion is due to the chemical potential of the aggressive agent:

$$q_i(\mathbf{x},t) = -\frac{D(T(\mathbf{x},t))}{RT(\mathbf{x},t)} c(\mathbf{x},t)\mu_{,i}(\mathbf{x},t) \tag{1}$$

in which, q_i denotes the components of the mass flux; D the diffusivity of the aggressive agent within the solid; T the temperature; R the universal gas constant; μ the chemical potential; and c the concentration of aggressive agent, given as the weight ratio of the diffusing agent and the solid substrate within an infinitesimal control volume. We adopt the index notation in the problem formulation (i.e., $i = 1, \ldots, n_{sd}$). Repeated indices of the spatial dimensions indicate summation unless otherwise stated. A subscript followed by a comma indicates partial derivative (i.e., $f_{,i} = \partial f/\partial x_i$). $\mathbf{x}$ and t parameterize the spatial and temporal dimensions, respectively. Bold symbol indicates vector notation (i.e., $\mathbf{x} = [x_1, x_2, x_3]$ for $n_{sd} = 3$). The chemical potential is a function of the concentration and the state of stress:

$$\mu(\mathbf{x},t) = \mu_0 + RT\,\ln(c) - \overline{V}_c p(\mathbf{x},t) \tag{2}$$

where μ_0 denotes the chemical potential at the stress free state and at equilibrium concentration; $p = -\sigma_{ii}/3$ denotes the pressure; $\overline{V}_c$ the partial molar volume of the ingressed gas in the substrate solid; and σ_i the components of the stress tensor. Using Eqs. (1) and (2), the transport equation of the stressed solid is given as

$$\dot{c} - (Dc_{,i})_{,i} - \left(\frac{Dc\overline{V}_c}{RT} p_{,i}\right)_{,i} = 0 \tag{3}$$

with superscribed dot indicates differentiation with respect to time. The initial and boundary conditions for the transport problem are expressed as

$$c(\mathbf{x}, t=0) = c_\infty(\mathbf{x}); \quad \mathbf{x} \in \Omega \tag{4}$$

$$c(\mathbf{x},t) = c_0(\mathbf{x},t); \quad \mathbf{x} \in \Gamma_D^c \tag{5}$$

$$q_i n_i(\mathbf{x},t) = 0; \quad \mathbf{x} \in \Gamma_N^c \tag{6}$$

in which, c_∞ is the concentration of the aggressive agent at the natural state of the solid; c_0 is the boundary concentration prescribed along $\Gamma_D^c \subset \Gamma$; $\Gamma_D^c \cap \Gamma_N^c = \varnothing$ and $\Gamma_D^c \cup \Gamma_N^c = \Gamma$; and, n_i are the components of the unit normal vector. Only homogeneous type Neumann boundary condition is considered for simplicity of the ensuing formulation, but the formulation can be extended to arbitrary Neumann or Robin conditions.

The transport process is coupled to the mechanical deformation through two mechanisms. The first is the stress-dependent chemical potential of the aggressive agent, which leads to the third term in the transport equation (Eq. (3)). The second is by linking the diffusivity to the state of damage within the solid. The effect of microcracking and damage on diffusivity has been recognized in geological materials, concrete and metals (e.g., [10–12]). The diffusivity is assumed to be enhanced as a function of the defect density (e.g. microcrack) as proposed by Krajcinovic [12]. The effect of evolving defect density on diffusivity is modeled based on the percolation theory [6] as

$$D(\omega, T) = D_0(1 + \mathcal{D}(\omega)) \exp\left(-\frac{Q}{RT}\right) \tag{7}$$

where D_0 is the pre-exponential constant; Q is the activation energy; and, $\mathcal{D}(\omega)$ is the effect of mechanical damage on