An one dimensional coupled model for deformation, degradation and solute diffusion in elastic solids

Fernando P. Duda
Universidade Federal do Rio de Janeiro - COPPE-PEM, RJ – Brazil
Angela C. Souza
Universidade Federal Fluminense - PGMEC-LMTA, RJ – Brazil
Leonardo J. Guimarães and Jose M. Barbosa
Universidade Federal de Pernambuco - CTG, PE – Brazil

Abstract

This paper deals with the formulation and numerical implementation of an one dimensional continuum model for deformation, degradation and solute diffusion in elastic solids. The formulation is carried out within the framework of continuum mechanics, where, in addition to the standard fields, extra fields are introduced in order to describe diffusion and damage processes. The governing equations are then obtained after supplementing the basic balances with a thermodynamically consistent constitutive theory. The couplings are implemented via the free energy response and include both deformation and damage assisted diffusion. It is worth mentioning that a gradient damage theory is obtained, which allows for the modelling of localization problems. The numerical implementation is based on the finite element method and a Euler implicit scheme for spatial and temporal discretizations, respectively. A numerical algorithm is presented to solve the discrete system of equations. In order to illustrate the potentiality of the proposed model, applications in the context of hydrogen assisted degradation are presented.

Keywords: continuum mechanics, solute diffusion in solids, hydrogen assisted degradation.

1 Introduction

Hydrogen assisted degradation is a phenomenon by which atomic hydrogen within a solid affects its mechanical properties in a deleterious fashion leading, eventually, to premature, and sometimes catastrophic, failure. It is a very important subject not only because of the ubiquity of hydrogen, which can be readily introduced in a component during its manufacture or service, but also because most high strength alloys are highly susceptible to the mentioned phenomenon. The study of hydrogen assisted degradation is very challenging once that multiple and coupled physical processes are involved, such

Mechanics of Solids in Brazil 2007, Marcílio Alves & H.S. da Costa Mattos (Editors)
Brazilian Society of Mechanical Sciences and Engineering, ISBN 978-85-85769-30-7

as diffusion, deformation and damage. There is no consensus regarding the damage mechanisms and two main candidates are the Hydrogen Enhanced Decohesion and the Hydrogen Enhanced Localized Plasticity. An excellent review on hydrogen assisted degradation can be found in Gangloff [1].

Motivated by the aforementioned problem in the context of the decohesion mechanism, we develop in this paper an one dimensional continuum model, along with its numerical implementation, for degradation and interstitial solute diffusion in elastic solids. Chemical reactions are neglected as well as thermal effects.

The model is developed within the framework of continuum mechanics. Accordingly, we first consider the kinematics where in addition to the standard field y, which describes the macroscopic motion of the solid, we introduce the microstructural fields d, c and J, where: d is the damage measure, which varies from 0 (pristine material) to 1 (cracked-up material); c is the solute concentration; J is the solute flow, which represents the local motion of the solute relative to the motion of the underlying solid. Then, using the Principle of Virtual Power, we introduce four balanced force systems: the standard or macroscopic force system, which expends power during macroscopic motion; the microforce systems, which expend power during changes in the microstructural fields. The basic balances of the theory are the force balances and the mass balance for the solute. We also consider as basic a mechanical version of the Second Law (the dissipation inequality), where the notion of chemical potential is introduced. After introducing a constitutive theory consistent with the dissipation inequality, the governing equations for y, d and J are obtained. The governing equation for c is obtained from the solute conservation equation. The following couplings, which are implemented via the free energy response, are obtained: stress and damage assisted diffusion and the accompanying composition induced stress and damage. The theory can account for: rate and non-local damage effects; non-fickian diffusion effects such as non-local and strain driven diffusion. It is obtained a simplified version of the theory, which will be the starting point for the numerical model.

To obtain the numerical model we begin by writing the coupled system of equations of the simplified theory in its weak version. Then, the temporal discretization is performed by means of the backward Implicit Euler Method. The resulting system of coupled equations are decoupled by using a staggered scheme. Finally, the Finite Element Method is used to perform the spatial discretization, where linear elements are used.

Two numerical examples are shown in order to illustrate the capability of the model to account for solute induced deformation, solute assisted degradation, deformation enhanced diffusion, deformation induced degradation, deformation induced and solute assisted degradation.

The developed model is an one dimensional version of the presented by the authors in Duda et all, 2003 [2].

This paper is organized as follows. In Section 2 it is formulated the general continuum theory. A specialized version of the general theory is presented in Section 3. Numerical implementation of the resulting equations is discussed in Section 4, while some numerical results are reported in Section 5. Finally, some concluding remarks are addressed in Section 6.

2 General theory

In this section we formulate a general theory for elasticity coupled with damage and diffusion within the framework of modern continuum mechanics.

2.1 Kinematics

We identify a body $\Omega := (0, L)$, $L > 0$, with the region of space it occupies in a fixed reference configuration. We denote by $\mathcal{D} := (x_1, x_2)$, $0 < x_1 < x_2 < L$, a typical part of Ω. Unless stated otherwise, by a field f we mean a spacetime field, and its temporal and spatial derivatives are denoted by $\dot{f} := \dfrac{\partial f}{\partial t}$ and $f_x := \dfrac{\partial f}{\partial x}$, respectively. The standard kinematic is described by the motion y such that $\lambda := y_x > 0$. The displacement u and the strain ϵ are defined as:

$$u(x,t) := y(x,t) - x, \quad \epsilon(x,t) := u_x = \lambda - 1. \tag{1}$$

In order to describe damage and solute diffusion, we assign to Ω the following extra kinematical descriptors: the damage measure d, which varies between zero (undamage) and 1 (completely damage); the solute concentration c, and the solute flux J, representing the local motion of the solute relative to the motion of the underlying solid. The corresponding realizable velocities are given by the list $V = (\dot{y}, \dot{d}, \dot{c}, J)$. By a generalized virtual velocity $\bar{V}$ we mean the list $(\bar{y}, \bar{d}, \bar{c}, \bar{J})$ of smooth fields on Ω. It is assumed that the space of all virtual velocities $\mathcal{V}$ contains, for a fixed time, the realizable velocity V.

2.2 Principle of virtual power

For given virtual velocity $\bar{V}$, the external and internal power expended on $\mathcal{D} \subset \Omega$ are defined, respectively, by:

$$P_e(\mathcal{D}, \bar{V}) := \int_{\mathcal{D}} (b\,\bar{y} + \pi^e \bar{d} + \gamma^e \bar{c} + \Upsilon^e \bar{J})\,\mathrm{dx} \tag{2}$$

and

$$P_i(\mathcal{D}, \bar{V}) := -\int_{\mathcal{D}} (N\,\bar{y}_x + \Pi\,\bar{d}_x + \pi^i \bar{d} + \Gamma \bar{c}_x + \gamma^i \bar{c} + \Sigma \bar{J}_x + \Upsilon^i \bar{J})\,\mathrm{dx}. \tag{3}$$

In the above equations, four independent force systems were introduced: i) the standard or macroscopic force system, which was described by the macro stress N and by the body force b; ii) the damage microforce system, which was characterized by the micro stress Π, by the external and internal microforce π^e and π^i, respectively; iii) the microforce system associated with the solute concentration c, which was characterized by the micro stress Γ, by the external and internal microforce γ^e and γ^i, respectively; iv) the microforce system associated with the solute flow J, which was is characterized by the micro stress Σ, by the external and internal microforce Υ^e and Υ^i, respectively. Inertial effects can be included in the external body forces.

The Principle of Virtual Power states that, for at each fixed time:

$$P_i(\mathcal{D},\bar{V}) + P_e(\mathcal{D},\bar{V}) = 0 \quad \forall\ \bar{V} \in \mathcal{V}. \tag{4}$$

Then, by using standard arguments, it follows from (4) that the following equations

$$\begin{aligned} & N_x + b = 0 \\ & \Pi_x - \pi^i + \pi^e = 0 \\ & \Gamma_x - \gamma^i + \gamma^e = 0 \\ & \Sigma_x - \Upsilon^i + \Upsilon^e = 0 \end{aligned} \tag{5}$$

must hold on Ω.

2.3 Mass balance and dissipation inequality

The local form of the mass balance for the solute states that:

$$\dot{c} = -J_x + h \quad \text{in} \quad \Omega, \tag{6}$$

where h the solute supply rate. Within the present context, the Second Law takes the form:

$$\frac{\mathrm{d}}{\mathrm{dt}}\int_{\mathcal{D}} \psi \,\mathrm{dx} \ \leq\ P_e(\mathcal{D},V) + \int_{\mathcal{D}} \mu\, h \,\mathrm{dx}, \tag{7}$$

where ψ is the free energy per unit of referential length and μ is the chemical potential. In the above inequality the left hand side represents the variation of the free energy in $\mathcal{D}$ per unit of time. The right hand side represents the energy supply due to external agencies. After using (4) and (6), the local form of the inequality (7) is given by:

$$\dot{\psi} \leq N\,\dot{u}_x \,+\, \Pi\,\dot{d}_x \,+\, \pi^i\dot{d} \,+\, \Gamma\,\dot{c}_x \,+\, (\gamma^i + \mu)\dot{c} \,+\, (\Sigma + \mu)J_x \,+\, \Upsilon^i J. \tag{8}$$

2.4 Constitutive theory

Following the dissipation inequality (8), we consider constitutive equations for the quantities:

$$\begin{aligned} & \psi = \hat{\psi}(\mathsf{e},\mathsf{n}), \quad N = \hat{N}(\mathsf{e},\mathsf{n}), \quad \Pi = \hat{\Pi}(\mathsf{e},\mathsf{n}), \quad \pi^i = \hat{\pi}(\mathsf{e},\mathsf{n}), \quad \Gamma = \hat{\Gamma}(\mathsf{e},\mathsf{n}), \\ & \gamma := \gamma^i + \mu = \hat{\gamma}(\mathsf{e},\mathsf{n}), \quad \Sigma + \mu = \hat{\Sigma}(\mathsf{e},\mathsf{n}), \quad \Upsilon^i = \hat{\Upsilon}(\mathsf{e},\mathsf{n}), \end{aligned} \tag{9}$$

where $\mathsf{e} := (\epsilon, d, d_x, c, c_x)$ and $\mathsf{n} := (J, \dot{d})$ represent equilibrium and non-equilibrium quantities, respectively. Therefore, the only dissipative processes considered are the damage and diffusion ones. From now on we assume that: the damage is irreversible, i.e, $\dot{d} \geq 0$, and the response function $\hat{\pi}$ is singular at $\dot{d} = 0$, which means that π is not constitutively defined when $\dot{d} = 0$.

Restrictions provided by the Dissipation Principle can be obtained via the Coleman-Noll procedure (see Silhavy, 1997 [3]). For the case we are concerned here, it can be shown that the aforementioned restrictions are the following:

i) Equilibrium relations:

$$\psi(\mathsf{e},\mathsf{n}) = \psi(\mathsf{e}), \quad \hat{N} = \frac{\partial\hat{\psi}}{\partial u_x}, \quad \hat{\Pi} = \frac{\partial\hat{\psi}}{\partial d_x}, \quad \hat{\Gamma} = \frac{\partial\hat{\psi}}{\partial c_x}, \quad \hat{\gamma} = \frac{\partial\hat{\psi}}{\partial c}, \quad \hat{\Sigma} = 0; \tag{10}$$

ii) Reduced dissipation inequality:

$$\hat{\pi}_d(\mathsf{e},\mathsf{n})\,\dot{d} + \hat{\Upsilon}(\mathsf{e},\mathsf{n})\,J \geq 0, \quad \text{where} \quad \hat{\pi}_d := \hat{\pi} - \frac{\partial\hat{\psi}}{\partial d}. \tag{11}$$

Therefore, the theory is constitutively specified by choosing the response functions $\hat{\psi}$, $\hat{\pi}_d$ and $\hat{\Upsilon}$, the latter two consistent with the inequality $(11)_1$. As we assume each term of the inequality $(11)_1$ non-negative, the most general representation for $\hat{\pi}_d$ and $\hat{\Upsilon}$ are given by:

$$\hat{\pi}_d(\mathsf{e},\mathsf{n}) = \hat{\pi}_1(\mathsf{e},J) + \hat{\pi}_2(\mathsf{e},\mathsf{n})\,\dot{d}, \quad \hat{\Upsilon}(\mathsf{e},\mathsf{n}) = \hat{H}(\mathsf{e},\mathsf{n})J, \tag{12}$$

In addition, we assume that $\hat{\pi}_2$ and $\hat{H}$ do not depend on $\dot{d}$ and J, respectively. Therefore, the reduced dissipation inequality is satisfied if and only if $\hat{\pi}_1 \geq 0$, $\hat{\pi}_2 \geq 0$ and $\hat{H} \geq 0$.

After combining the constitutive information introduced so far (equations $(9)_4$, $(10)_3$, $(11)_2$ and $(12)_1$) with the balance equation $(5)_2$, we have:

$$\hat{\pi}_2(\mathsf{e},\mathsf{n})\,\dot{d} = -\delta_d\hat{\psi}(\mathsf{e}) - \hat{\pi}_1(\mathsf{e},J) + \pi^e, \quad \text{where} \quad \delta_d\hat{\psi} := \frac{\partial\hat{\psi}}{\partial d} - \frac{\partial}{\partial x}\left(\frac{\partial\hat{\psi}}{\partial d_x}\right) \tag{13}$$

is the variational derivative of $\hat{\psi}$ with respect to d. Equation (13) constrains the manner in which damage occurs and provides that

$$-\delta_d\hat{\psi}(\mathsf{e}) - \hat{\pi}_1(\mathsf{e},J) + \pi^e > 0 \tag{14}$$

is a necessary condition for damage growth. We assume that (14) is also sufficient for damage growth.

2.5 Summary of the governing equations

To obtain the governing equations of the theory we combine the basic balances, namely force balances and solute mass conservation, with a constitutive theory compatible with the dissipation inequality. In addition, it should be provided appropriate boundary and initial conditions as well as prescriptions for: the response functions $\hat{\psi}$, $\hat{\pi}_1$, $\hat{\pi}_2$ and $\hat{H}$; the external force densities b, π^e, γ^e and Υ^e. We summarize the governing equations of the theory as follows. We have three partial differential equations for the fields u, d and c:

i) Standard force balance (equations $(5)_1$ and $(10)_2$):

$$\frac{\partial}{\partial x}\left(\frac{\partial\hat{\psi}}{\partial u_x}\right)+b=0; \tag{15}$$

ii) Damage force balance (equation (13)):

$$\hat{\pi}_2(\mathsf{e},\mathsf{n})\,\dot{d}=<-\delta_d\hat{\psi}(\mathsf{e})-\hat{\pi}_1(\mathsf{e},J)+\pi^e>,\quad \delta_d\hat{\psi}:=\frac{\partial\hat{\psi}}{\partial d}-\frac{\partial}{\partial x}\left(\frac{\partial\hat{\psi}}{\partial d_x}\right), \tag{16}$$

where <> is the Macauley bracket;

iii) Solute conservation equation (equation (6)):

$$\dot{c}=-J_x+h. \tag{17}$$

The equation (17) must be supplemented with the definition of the solute flow and the chemical potential, which are obtained from the remaining two extra force balances:

iv) Solute flow force balance (equations $(5)_4$, $(9)_7$, $(10)_6$ and $(12)_2$) :

$$\hat{H}(\mathsf{e},\mathsf{n})J=-\mu_x+\Upsilon^e; \tag{18}$$

v) Solute force balance (equations $(5)_3$, $(9)_6$ and $(10)_{4,5}$) :

$$\mu=\delta_c\hat{\psi}(\mathsf{e})-\gamma^e,\quad \delta_c\hat{\psi}:=\frac{\partial\hat{\psi}}{\partial c}-\frac{\partial}{\partial x}\left(\frac{\partial\hat{\psi}}{\partial c_x}\right). \tag{19}$$

3 Special theory

In this section a simplified version of the theory is presented. Firstly we suppose a supply rate given by:

$$h=p\,q\,(c-c_{eq}) \tag{20}$$

where c_{eq} is the solute concentration in the equilibrium state, p is the cross area perimeter and q is the surface limited mass transfer coefficient, that can account for all surface effects, including roughness for instance. We also assume that $\pi^e=\gamma^e=\Upsilon^e=0$, and that all the couplings are implemented via the free energy response $\hat{\psi}$. The following constitutive choices are then adopted:

i) Free energy response:

It is assumed the following additive decomposition for the free energy response

$$\hat{\psi}(\epsilon, d, c, d_x) = \hat{\varepsilon}(\epsilon, d, c) + dAw(1 - \lambda c) + \alpha A(\ln c - 1)c + \frac{\kappa A}{2} {d_x}^2, \tag{21}$$

where $\epsilon = u_x$ is the strain, w, λ, α and κ are positive material constants, and A is the cross sectional area. The strain energy response $\hat{\varepsilon}$ is given by:

$$\hat{\varepsilon}(\epsilon, d, c) = \frac{1-d}{2} E \, A \, \epsilon_e, \quad \text{where} \quad \epsilon = \epsilon_e + e(c - c_{rf}) \tag{22}$$

is the additive decomposition of the strain into its elastic and chemical parts, E is the elasticity modulus, c_{rf} is a reference solute concentration and e a positive material constant;

ii) Dissipative responses:

$$\hat{\pi}_1(\mathsf{e}, J) = 0, \quad \hat{\pi}_2(\mathsf{e}, \mathsf{n}) = \beta \, A, \quad \hat{H}(\mathsf{e}, \mathsf{n}) = \frac{A}{cM}, \tag{23}$$

where β and M are positive parameters.

With the above assumptions, the linear elasticity coupled with damage and diffusion problem can be stated as follows:

Given: Boundary/initial conditions, material and geometrical parameters, body force density, reference and equilibrium concentration,
Find: The displacement u, the damage d and the concentration c, satisfying the following equations:

$$\begin{cases} N_x + b = 0, \quad N = EA(1-d)(u_x - e\,(c - c_{rf})) \\ J_x + \dot{c} = p\,q\,(c - c_{eq}), \quad J = -D\,c_x + \dfrac{D}{\alpha} c \left(w \lambda \, d_x - \dfrac{e}{A} \, b \right), \ D = \alpha \, M \\ \beta \, \dot{d} = < \dfrac{E}{2}(u_x - e\,(c - c_{rf}))^2 - w\,(1 - \lambda c) + \kappa \, d_{xx} > \end{cases} \tag{24}$$

The relation $(24)_1$ shows that the elastic properties are modified by the presence of damage and the second term of its right hand side represents the composition induced stress. The relation $(24)_2$ shows that diffusion is driven by concentration, hydrostatic stress and damage gradients. It shows that the solute flows from a region of higher to region of lower concentration. The opposite effect occurs with respect to both hydrostatic stress and damage. The relation $(24)_3$ shows that damage driving force is the stored energy of the virgin material whereas the damage resistance is composed by two contributions. The local contribution depends on the solute concentration: the higher the solute concentration, the lower is the damage resistance.

4 Numerical model

In this section the computational model corresponding to the equations (24) is obtained. The starting point for the formulation of the numerical method consists in writing these governing equations in their weak forms, as described as follows:

Given: Boundary/initial conditions, material and geometrical parameters, body force density and reference concentration,
Find: $\{c, u, d\} : [0, L] \times [0, T] \mapsto \Re$
Such that:

$$\begin{aligned} &\int_0^L (J\,\varphi_x - \dot{c}\,\varphi + h\,\varphi)\,\mathrm{dx} = 0 \quad \forall\ \varphi\ \in\ V^0 \\ &\int_0^L (N\,v_x - b\,v)\,\mathrm{dx} = 0 \quad \forall\ v\ \in\ V^0 \\ &\int_0^L (\Pi\,\gamma_x + \pi\,\gamma)\,\mathrm{dx} = 0 \quad \forall\ \gamma\ \in\ V^0 \end{aligned} \tag{25}$$

where:

$$\begin{aligned} &V^0 = \{f : [0, L] \mapsto \Re, \text{ sufficiently smooth, } f(0) = f(L) = 0\} \\ &J = -D\,c_x + \frac{D}{\alpha} c \left(w\lambda\, d_x - \frac{e}{A} b \right), \quad h = p\,q\,(c - c_{eq}) \\ &N = EA(1 - d)(u_x - e\,(c - c_{rf})) \\ &\Pi = \kappa\, d_x, \quad \pi = \beta \dot{d} - \frac{E}{2}(u_x - e(c - c_{rf}))^2 + w(1 - \lambda c) \end{aligned} \tag{26}$$

For the sake of notation simplicity, possible boundary contributions were omitted throughout this work, although have been accounted in the numerical model.

A backward Euler scheme is adopted for the temporal discretization, consequently the supercripts k refers to time instant t_k, and $\dot{f}^k = \dfrac{f^k - f^{k-1}}{t_k - t_{k-1}}$, where $f^k = f(t_k)$. The operator splitting method was used to solve the coupled equations systems (25), so that, at first c^k is calculated in $(25)_1$ by considering d^k obtained in the previous time step; then u^k is calculated in $(25)_2$ by considering d^k and c^k obtained before, and finally d^k is obtained in $(25)_3$ by using u^k and c^k already obtained. Then, the equations (25) become:

Given: Boundary/initial conditions, material and geometrical parameters, body force density, reference concentration and $\mathcal{T} = \{t_0 = 0, t_1, ..., t_{k-1}, t_k, ...t_N = T\}$
Find, for k = 1, N: $\{c^k, u^k, d^k\} : [0, L] \mapsto \Re$

Such that, for k = 1, N:

$$
\begin{aligned}
&\mathcal{A}_c^k(c^k,\varphi;d^{k-1}) = \mathcal{L}_c^k(\varphi;c^{k-1}) \quad \forall\, \varphi \;\in\; V^0\\
&\mathcal{A}_u^k(u^k,v;d^{k-1}) = \mathcal{L}_u^k(v;d^{k-1},c^k) \quad \forall\, v \;\in\; V^0\\
&\mathcal{A}_d^k(d^k,\gamma) = \mathcal{L}_d^k(\gamma;d^{k-1},u^k,c^k) \quad \forall\, \gamma \;\in\; V^0
\end{aligned} \tag{27}
$$

where:

$$
\begin{aligned}
&\mathcal{A}_c^k(c^k,\varphi;d^{k-1}) = \int_0^L \left(-D\,c_x^k\,\varphi_x + \frac{D}{\alpha}c^k\left(w\,\lambda\,d_x^{k-1} - \frac{e}{A}b\right)\varphi_x - \frac{c^k}{\Delta t}\varphi + p\,q\,c^k\varphi\right)\,\mathrm{dx}\\
&\mathcal{L}_c^k(\varphi;c^{k-1}) = \int_0^L \left(-\frac{c^{k-1}}{\Delta t}\,\varphi + p\,q\,c_{eq}\,\varphi\right)\,\mathrm{dx}\\
&\mathcal{A}_u^k(u^k,v;d^{k-1}) = \int_0^L EA\,(1-d^{k-1})\,u_x^k\,v_x\,\mathrm{dx}\\
&\mathcal{L}_u^k(v;d^{k-1},c^k) = \int_0^L (eEA\,(1-d^{k-1})\,(c^k-c_{rf})\,v_x - b\,v)\,\mathrm{dx}\\
&\mathcal{A}_d^k(d^k,\gamma) = \int_0^L \left(\kappa\,d_x^k\,\gamma_x + \beta\,\frac{d^k}{\Delta t}\,\gamma\right)\,\mathrm{dx}\\
&\mathcal{L}_d^k(\gamma;d^{k-1},u^k,c^k) = \int_0^L \left(\beta\,\frac{d^{k-1}}{\Delta t}\,\gamma + \frac{E}{2}(u_x^k - e(c^k-c_{rf}))^2\gamma + w\,(1-\lambda c^k)\gamma\right)\,\mathrm{dx}
\end{aligned} \tag{28}
$$

Observe that $\mathcal{A}_c^k$ is bilinear in c^k, $\mathcal{A}_u^k$ is bilinear in u^k and $\mathcal{A}_d^k$ is bilinear in d^k, whereas $\mathcal{L}_c^k$ is linear in φ, $\mathcal{L}_u^k$ is linear in v and $\mathcal{L}_d^k$ is linear in γ.

In the setting of the finite element method, the solution and test spaces are approximated by finite dimensional spaces. Therefore, we denoted V^{0h} the space of the test functions, satisfying the homogeneous boundary conditions, and V^h the space of the solutions functions, satisfying the real boundary conditions. The test functions are denoted by: φ_h, v_h and γ_h belonging to V^{0h}, and the approximated solution fields are denoted by c_h, u_h and d_h belonging to V^h. The weighting functions (Ψ) are chosen according to Galerkin method, and as a result of this discretization, the equation (27) can be written as a summation over all elements, where $\mathbf{c}_h$, $\boldsymbol{u}_h$, $\mathbf{d}_h$, $\mathbf{f}_h$, $\mathbf{v}_h$ and $\mathbf{g}_h$ are vectors of the nodal values related with the functions c_h, u_h, d_h, φ_h, v_h and γ_h.

For each time instant $t_k, k = 1, N$:

$$
\begin{aligned}
&\boldsymbol{M}_k\mathbf{c}_h^k\cdot\mathbf{f}_h = \mathbf{G}_k\cdot\mathbf{f}_h, \quad \forall\ \mathbf{f}_h \in\ \Re^{ne-1}\\
&\boldsymbol{K}_k\boldsymbol{u}_h^k\cdot\mathbf{v}_h = \boldsymbol{F}_k\cdot\mathbf{v}_h, \quad \forall\ \mathbf{v}_h \in\ \Re^{ne-1}\\
&\mathbf{L}_k\mathbf{d}_h^k\cdot\mathbf{g}_h = \mathbf{H}_k\cdot\mathbf{g}_h, \quad \forall\ \mathbf{g}_h \in\ \Re^{ne-1}
\end{aligned} \tag{29}
$$

where ne is the number of elements, and:

$$\begin{aligned} (\boldsymbol{M}_k)_{ij} &= \mathcal{A}_c^k(\Psi_i, \Psi_j), \quad (\mathbf{G}_k)_i = \mathcal{L}_c^k(\Psi_i) \\ (\boldsymbol{K}_k)_{ij} &= \mathcal{A}_u^k(\Psi_i, \Psi_j), \quad (\boldsymbol{F}_k)_i = \mathcal{L}_u^k(\Psi_i) \\ (\mathbf{L}_k)_{ij} &= \mathcal{A}_d^k(\Psi_i, \Psi_j), \quad (\mathbf{H}_k)_i = \mathcal{L}_d^k(\Psi_i) \end{aligned} \tag{30}$$

for $i, j = 1, (ne - 1)$.

The resulting algorithm is described as follows:

- Given: Boundary conditions, material and geometrical parameters, body force density, reference and equilibrium concentration
- Initializations: $t_k = 0,\ u(x,0) = u_0(x),\ d(x,0) = d_0(x),\ c(x,0) = c_0(x),\ k = 1$
- For each time step $t_k \leq T$
  - By calculating $\boldsymbol{M}_k$ and $\mathbf{G}_k$, obtain $\mathbf{c}^k$: $\boldsymbol{M}_k\mathbf{c}^k = \mathbf{G}_k$
  - By calculating $\boldsymbol{K}_k$ and $\boldsymbol{F}_k$, obtain $\boldsymbol{u}^k$: $\boldsymbol{K}_k\boldsymbol{u}^k = \boldsymbol{F}_k$
  - By calculating $\mathbf{L}_k$ and $\mathbf{H}_k$, obtain $\mathbf{d}^k$: $\mathbf{L}_k\mathbf{d}^k = \mathbf{H}_k$
  - Update: $k = k + 1$ and return

5 Numerical examples

The numerical results presented in this section illustrate the capabilities of the proposed model as well as the performance of the corresponding algorithm. Two problems involving transport of hydrogen in a cylindrical rod (length 100 mm and cross section diameter 3 mm) of AISI 4340 steel were used. Standard material properties are: the parameter $E = 2.0\text{x}10^{11}$ Pa is the elasticity modulus. The parameters associated with the solute are: the diffusion coefficient $D = 1.0\text{x}10^{-10}$ m^2/s; $\alpha = \rho RT = 1.94\text{x}10^{10}$ J/m^3, where ρ is the density, T is the temperature and R is the gas constant; and the linear expansion coefficient for the hydrogen $e = 5.2$ (see for instance [4]). The parameters associated with the damage are: the parameter which measure the influence of damage at a material point on the damage of this neighbourhood $\kappa = 37.52$ Pa.m^2; the viscosity parameter $\beta = 1.0\text{x}10^3$ Pa.s; the initial damage threshold $w = 3.08\text{x}10^6$ Pa; and the coupling between damage and diffusion $\lambda = 35.0\text{x}10^4$.

In the first example the road is subject to a singular body force as can be seen in Figure 1. The boundary conditions used are:

$$J(x=0) = 0,\ u(x=0) = 0,\ \Pi(x=0) = 0,\ c(x=L) = 1.0\text{x}10^{-7},\ N(x=L) = 0,\ \Pi(x=L) = 0$$

where, according equation (25), J is the solute flow, c is the solute concentration, u is the displacement, N is the macro stress and Π is the microstress associated with the damage. In this example we consider the reference solute concentration (equation (22)) $c_{rf} = 1.0\text{x}10^{-7}$ and the supply rate (equation (20)) $h = 0$. The rod was discretized using 101 elements. A transient analysis was performed

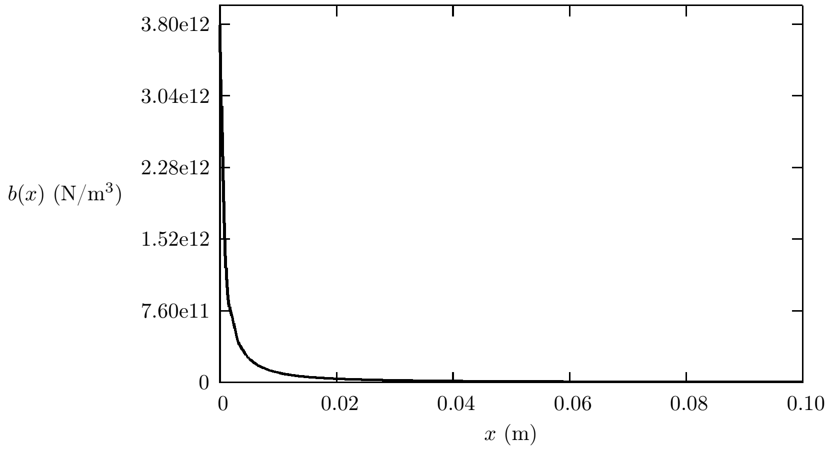

Figure 1: Applied body force in the first example

with the fully coupled model, and the Figures 2, 3 and 4 show the distribution of solute concentration, displacement and damage, respectively, at the time instants: $t_1 = 90.0\text{s}$, $t_2 = 5.1121224\text{x}10^7\text{s}$, $t_3 = 5.1121225\text{x}10^7\text{s}$, $t_4 = 5.1121226\text{x}10^7\text{s}$.

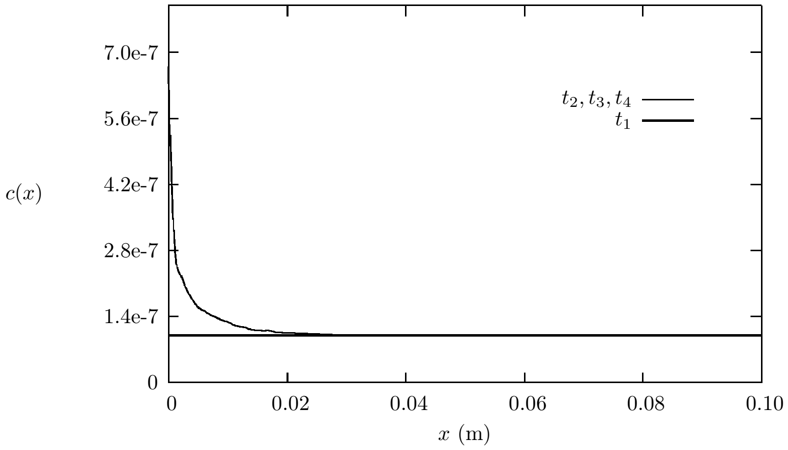

Figure 2: Distribution of solute concentration in the first example

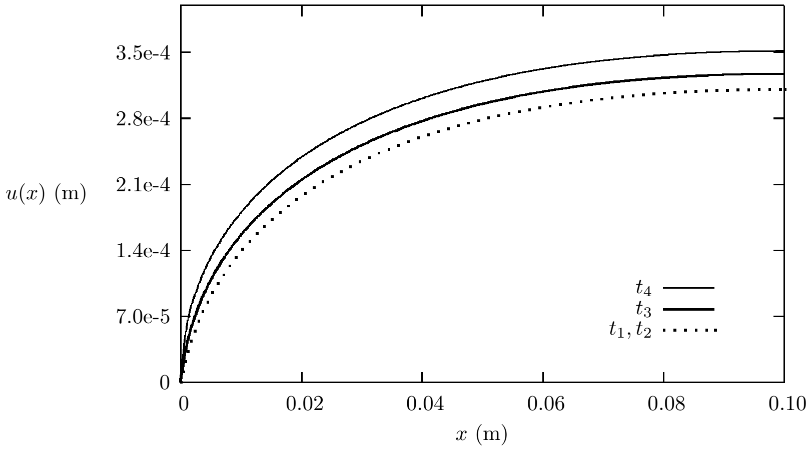

Figure 3: Displacement in the first example

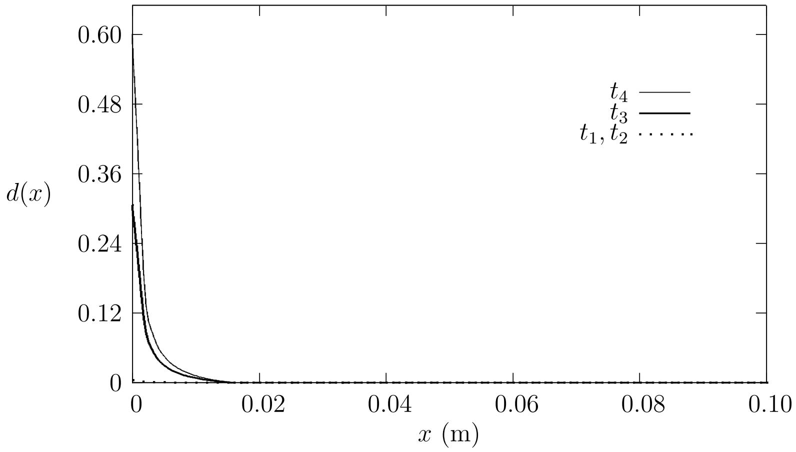

Figure 4: Distribution of damage in the first example

In the second example the road is subject to a singular supply rate as can be seen in Figure 5. The objective of this example is to simulate entrance of hydrogen throughout a defect in a surface of the road. The boundary conditions used are:

$$J(x=0)=0,\ u(x=0)=0,\ \Pi(x=0)=0,\ J(x=L)=0,\ N(x=L)=0,\ \Pi(x=L)=0$$

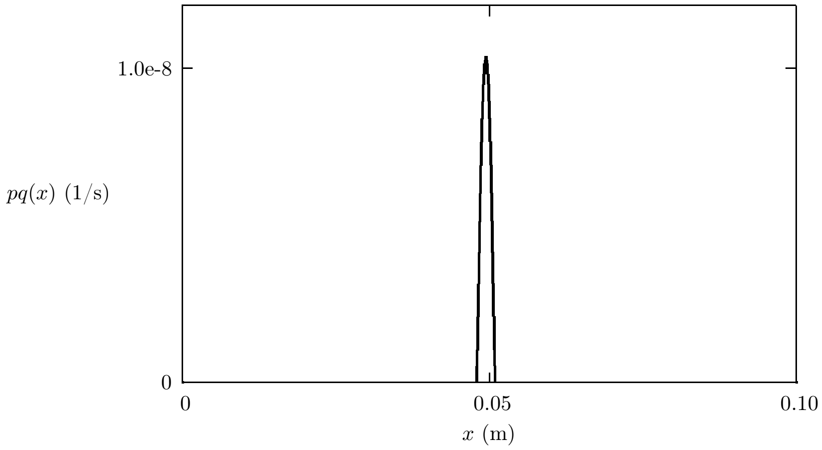

Figure 5: Supply rate in the second example

In this example we consider the reference solute concentration $c_{rf} = 0$, the equilibrium solute concentration $c_{eq} = 1.28$ and the body force $b = 0$. A transient analysis was performed with the fully coupled model, and the Figures 6, 7 and 8 show the evolution of the solute concentration, the displacement and the damage, respectively, at the time instants: $t_1 = 3.0\text{x}10^3$s, $t_2 = 1.5\text{x}10^3$s, $t_3 = 19.8\text{x}10^3$s, $t_4 = 22.2957\text{x}10^3$s, $t_5 = 22.2958\text{x}10^3$s, $t_6 = 22.2959\text{x}10^3$s.

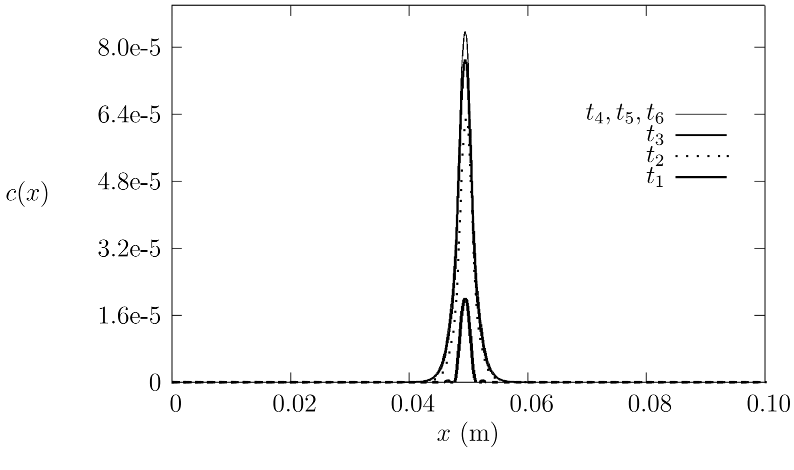

Figure 6: Distribution of solute concentration in the second example

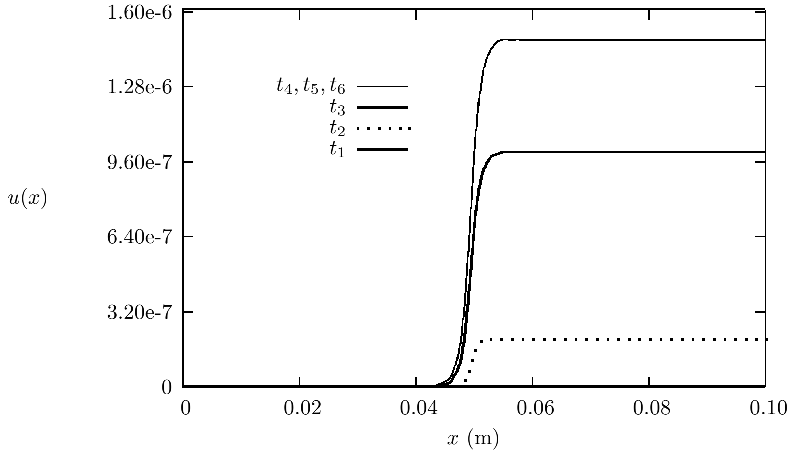

Figure 7: Displacement in the second example

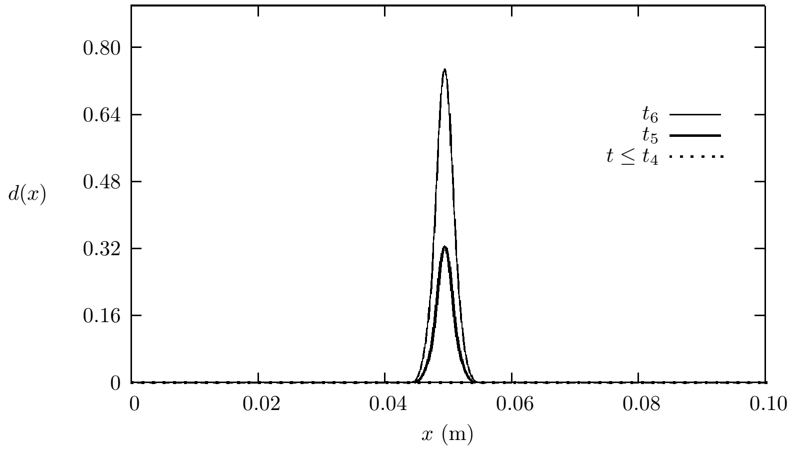

Figure 8: Distribution of damage in the second example

6 Conclusions

An one dimensional coupled continuum model for deformation, diffusion and damage in elastic solids was developed within the scheme of continuum mechanics. The following couplings were introduced: damage-deformation, in which the damage degrades the elastic properties; deformation-damage: in which the strain energy promotes degradation; diffusion-damage, in which the presence of the solute decreases the damage resistance; damage-diffusion, in which the damage enhances the diffusion; deformation-diffusion, in which the presence of the stress promotes the diffusion; diffusion-deformation, in which the solute induces a chemical stress. A numerical model of the simplified theory was developed. Two illustrative numerical examples were provided.

Acknowledgements

The first author gratefully acknowledges the support of this by the CNPq (350252/2000-9) and FAPERJ (E-26/171.599/2004).

References

[1] Gangloff, R., *Hydrogen Assisted Cracking of High Strength Alloys: Comprehensive Structural Integrity*, volume 6. Elsevier Science: New York, 2003.

[2] Duda, F., aes, L.G., Souza, A. & Barbosa, J., On the modeling of deformation-diffusion-damage coupling in elastic solids. *III European Conference on Computational Mechanics*, Lisboa, 2006.

[3] Silhavy, M., *he Mechanics and Thermodynamics of Continuous Media*. Springer-Verlag: Berlin, 1997.

[4] Thomas, J. & Chopin, C., Modeling of coupled deformation-diffusion in non-porous solids. *Int J Engineering Science*, **37**, pp. 1–24, 1999.