ON A THEORY OF ELASTICITY COUPLED WITH DAMAGE AND DIFFUSION

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Abstract. *This paper aims at the formulation and numerical implementation of a continuum theory for linear elasticity coupled with damage and diffusion. The continuum theory is described within the framework of continuum mechanics, in which the governing equations are obtained after combining the basic balances with a constitutive theory compatible with a mechanical version of the Second Law of Thermodynamics. The numerical implementation is based on the Implicit Euler Method and the Finite Element Method for the temporal and spatial discretization, respectively. It is used a staggered scheme to solve the resulting discrete model. Numerical examples are provided to illustrate the application of the theory and numerical scheme as well.*

Keywords: *continuum mechanics, damage, diffusion*

1. Introduction

In this paper we propose an one dimensional continuum theory, together with its corresponding numerical model, for deterioration in linearly elastic solids that accounts for the diffusion of a single solute. We assume that deterioration is the result of microscale processes such as nucleation, growth and coalescence of microcraks, which are promoted by mechanical loads on the macroscale. These processes may be influenced by the presence of the solute, which diffuses within the underlying solid. Chemical reactions are neglected as well as thermal effects.

We develop our theory 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, ρ and J, where: d is the damage measure, which varies from 0 (pristine material) to 1 (cracked-up material); ρ is the solute density; J, which represents the local motion of the solute relative to the motion of the underlying solid, is the solute flow. 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 are obtained. In particular, the governing equations for y, d and J are obtained from their corresponding force balances. The latter involves the chemical potential μ that is defined by the force balance associated to ρ. The governing equation for ρ is obtained from the solute conservation equation. 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. Numerical examples are provided to illustrate the application of the theory and the numerical scheme as well.

In some aspects, this paper extends the work presented by the authors in Duda et all (2003) and Duda and Souza (2004). The treatment of diffusion adopted here is akin to the one presented by Fried and Sellers (2000). For the relevance of the subject discussed in this paper see Thomas and Chopin (1997) and references cited therein.

This paper is organized as follows. Section 2 introduces the basic notions of a continuum theory for linear elasticity coupled with damage and diffusion. A general constitutive theory is presented in Section 3. A special theory is obtained in Section 4. Numerical implementation of the resulting equations is discussed in Section 5, while some numerical results are reported in Section 6. Finally, some concluding remarks are addressed in Section 7.

2. Basic Notions

We identify a body with its reference configuration $\Omega := (0, L)$, $L > 0$. 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 we mean a spacetime field. For a given field f, its temporal and spatial derivatives are denoted by $\dot{f} := \frac{\partial f}{\partial t}$ and $f_x := \frac{\partial f}{\partial x}$, respectively.

We assign to Ω the kinematical descriptors y, d, ρ and J, where: the motion y is such that $\lambda := y_x > 0$; the damage field d varies between zero (undamaged) and 1 (completely damaged), and ρ and J represent, respectively, the solute density and flow. The corresponding realizable velocities are given by the list $V = (\dot{y}, \dot{d}, \dot{\rho}, J)$. We observe that J is already a rate variable. Other quantities of interest are the displacement field u, defined by the relation $u(x,t) := y(x,t) - x$, and the strain $\epsilon := u_x = \lambda - 1$.

By a generalized virtual velocity $\mathcal{V}$ we mean the list $(v, \nu, \omega, \mathcal{J})$ of smooth fields on Ω. It is assumed that the space of all virtual velocities contains, for a fixed time, the realizable velocity V.

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

$$P_e(\mathcal{D}, \mathcal{V}) := \int_{\mathcal{D}} (bv + \pi^e \nu + \gamma^e \omega + \Upsilon^e \mathcal{J}) \, \mathrm{dx} + \sum_{i=1}^{2} (s(x_i)v(x_i) + g(x_i)\nu(x_i) + w(x_i)\omega(x_i) + Z(x_i)\mathcal{J}(x_i)), \quad (1)$$

and

$$P_i(\mathcal{D}, \mathcal{V}) := -\int_{\mathcal{D}} (N v_x + \Pi \nu_x + \pi^i \nu + \Gamma \omega_x + \gamma^i \omega + \Sigma \mathcal{J}_x + \Upsilon^i \mathcal{J}) \, \mathrm{dx}, \quad (2)$$

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, by external body force b and by the contact force s; ii) the damage microforce system, which was characterized by the micro stress Π, by the external and internal microforce π^i and π^e, respectively, and by the contact microforce g; iii) the microforce system associated with the density ρ, which was characterized by the micro stress Γ, by the external and internal microforce γ^i and γ^e, respectively, and by the contact microforce w; iv) the microforce system associated with J, which was is characterized by the micro stress Σ, by the external and internal microforce Υ^e and Υ^i, respectively, and by the contact microforce Z.

The Principle of Virtual Power states that, at each fixed time, for any generalized virtual velocity $\mathcal{V}$ and each part $\mathcal{D}$ of Ω,

$$P_i(\mathcal{D}, \mathcal{V}) + P_e(\mathcal{D}, \mathcal{V}) = 0. \quad (3)$$

Then, by using standard arguments, it follows from (1), (2) and (3) that

$$\left.\begin{array}{l} N_x + b = 0 \\ \Pi_x - \pi^i + \pi^e = 0 \\ \Gamma_x - \gamma^i + \gamma^e = 0 \\ \Sigma_x - \Upsilon^i + \Upsilon^e = 0 \end{array}\right\} \quad \text{in} \quad \mathcal{D}, \qquad \begin{array}{ll} s(x_1) = -N(x_1), & s(x_2) = N(x_2) \\ g(x_1) = -\Pi(x_1), & g(x_2) = \Pi(x_2) \\ w(x_1) = -\Gamma(x_1), & w(x_2) = \Gamma(x_2) \\ Z(x_1) = -\Sigma(x_1), & Z(x_2) = \Sigma(x_2) \end{array} \quad (4)$$

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

$$\dot{\rho} = -J_x + h \quad \text{in} \quad \Omega, \quad J(L,t) = q(L,t), \qquad J(0,t) = q(0,t), \quad (5)$$

where q is the solute flow across the boundary $\partial\Omega$ and h the solute supply rate.

Within the present context, the Second Law takes the form:

$$\frac{\mathrm{d}}{\mathrm{dt}} \int_{\mathcal{D}} \psi \, \mathrm{dx} \le P_e(\mathcal{D}, V) + \int_{\mathcal{D}} \mu \, h \, \mathrm{dx}, \quad (6)$$

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 (3) and (5), the local form of the inequality (6) is given by:

$$\dot{\psi} \le N\dot{\epsilon} + \Pi \dot{d}_x + \pi^i \dot{d} + \Gamma \dot{\rho}_x + (\gamma^i + \mu)\dot{\rho} + (\Sigma + \mu) J_x + \Upsilon^i J. \quad (7)$$

3. Constitutive Theory

Guided by the dissipation inequality (7), we consider constitutive equations for the quantities:

$$\psi = \hat{\psi}(\mathsf{p}), N = \hat{N}(\mathsf{p}), \Pi = \hat{\Pi}(\mathsf{p}), \pi^i = \hat{\pi}(\mathsf{p}), \Gamma = \hat{\Gamma}(\mathsf{p}), \; \gamma^i + \mu = \hat{\gamma}(\mathsf{p}), \; \Sigma + \mu = \hat{\Sigma}(\mathsf{p}), \Upsilon^i = \hat{\Upsilon}(\mathsf{p}) \quad (8)$$

with $\mathsf{p} := (\mathsf{e}, \mathsf{n})$, where $\mathsf{e} := (\epsilon, d, d_x, \rho, \rho_x)$ 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, $\dot{d} \geq 0$; the response function $\hat{\pi}$ is singular at $\dot{d} = 0$, which means that π is not constitutively determinated when $\dot{d} = 0$.

Now we obtain thermodynamic restrictions on the response functions by following the Coleman-Noll procedure. By omitting the details, the application of the aforementioned procedure delivers that:

$$\hat{\psi}(\mathsf{p}) = \hat{\psi}(\mathsf{e}), \quad \hat{N} = \frac{\partial \hat{\psi}}{\partial \epsilon}, \quad \hat{\Pi} = \frac{\partial \hat{\psi}}{\partial d_x}, \quad \hat{\Gamma} = \frac{\partial \hat{\psi}}{\partial \rho_x}, \quad \hat{\gamma} = \frac{\partial \hat{\psi}}{\partial \rho}, \quad \hat{\Sigma} = 0 \tag{9}$$

and the response functions $\hat{\pi}$ and $\hat{\Upsilon}$ must comply with the residual inequality:

$$\hat{\pi}_d(\mathsf{p})\, \dot{d} + \hat{\Upsilon}(\mathsf{p}) J \geq 0, \tag{10}$$

where $\hat{\pi}_d := \hat{\pi} - \frac{\partial \hat{\psi}}{\partial d}$.

Thus, from the constitutive point of view, the theory is completely specified by choosing the response functions $\hat{\psi}$, $\hat{\pi}_d$ and $\hat{\Upsilon}$. From now on we assume that: i) the free energy response given by

$$\hat{\psi}(\mathsf{e}) = \hat{w}(\epsilon, d, \rho) + \hat{\phi}(d, \rho, d_x, \rho_x), \quad \frac{\partial \hat{w}}{\partial d} \leq 0 \tag{11}$$

where $\hat{w}$ is the strain energy whereas $\hat{\phi}$ is the stored energy by the defects; ii) the dissipative responses $\hat{\pi}_d$ and $\hat{\Upsilon}$ are given by

$$\hat{\pi}_d(\mathsf{p}) = \hat{a}(\mathsf{e}, J) + \hat{b}(\mathsf{p})\, \dot{d}, \quad \hat{\Upsilon} = \hat{H}(\mathsf{p}) J, \tag{12}$$

where $\hat{a} \geq 0$, $\hat{b} > 0$ and $\hat{H} > 0$ in order to satisfy the reduced dissipation inequality (10).

From the balance equation $(4)_2$, and assuming that $\pi^e = 0$, we have

$$\hat{b}\, \dot{d} = \tau - r \quad \text{if} \quad \dot{d} > 0, \tag{13}$$

where:

$$\tau := -\frac{\partial \hat{w}}{\partial d} \geq 0 \quad \text{and} \quad r := -\left(\frac{\partial \hat{\phi}}{\partial d_x} \right)_x + \frac{\partial \hat{\phi}}{\partial d} + \hat{a}, \tag{14}$$

where τ is the damage driving force and r is the damage resistance. Thus, the former equation implies that the condition $\tau > r$ is necessary for damage growth. As an additional constitutive assumption, it is assumed that the aforementioned condition is also sufficient for damage growth.

Combining the constitutive theory developed so far and the micro force balances, we obtain:

i) the damage governing equation:

$$\hat{b}(\mathsf{p})\, \dot{d} = < \tau - r >, \tag{15}$$

where $<>$ is the Macauley bracket;

ii) the expression for the chemical potential:

$$\mu = \frac{\partial \hat{\psi}}{\partial \rho} - \left(\frac{\partial \hat{\psi}}{\partial \rho_x} \right)_x - \gamma^e; \tag{16}$$

iii) the expression for the mass flow:

$$\hat{H}(\mathsf{p}) J = -\mu_x + \Upsilon^e. \tag{17}$$

4. Special Theory

In this section a simplified version of the theory is presented. In this context, it is assumed that: the deformation-diffusion and deformation-damage couplings are implemented in the free energy; the damage-diffusion coupling is implemented in the dissipative response $\hat{\pi}_d$. Thus, the following constitutive assumptions are adopted:

i) the free energy is given by:

$$\psi(\varepsilon, d, \rho, d_x) = \underbrace{\frac{E}{2}(1-d)(\varepsilon - e\rho)^2}_{\hat{w}} + \underbrace{\frac{c}{2}\rho^2 + \frac{\kappa}{2}(d_x)^2}_{\hat{\phi}}, \tag{18}$$

E is the elasticity modulus, A the cross sectional area, and e, c and κ are positive material parameters. Thus, N and μ reduce to

$$N = (1-d)EA(\varepsilon - e\rho), \quad \mu = -e(1-d)EA(\varepsilon - e\rho) + c\rho = -eN + c\rho. \tag{19}$$

The former expression accounts for composition induced stress;

ii) the dissipative responses are determined by

$$\hat{a}(\mathsf{e}, J) =< w(1-\lambda\rho) >, \quad \hat{b}(\mathsf{p}) = b, \quad \hat{H} = \frac{1}{M}, \tag{20}$$

where w, λ, b and M are positive parameters. From the expression for $\hat{a}$ we see that the damage resistance is a non-increasing function of the solute density. So, the solute may represent a corrosive substance in this case. In the opposite case, the solute could represent a healing substance.

With these assumptions, it follows from (16) and (17) that

$$J = -D\left(\rho_x - \frac{e}{c}N_x\right), \tag{21}$$

where $D := cM$ is the diffusion coefficient. Thus, by using the equation (5) and assuming $h = 0$, the governing equation for the solute density is given by

$$\dot{\rho} = D\left(\rho_{xx} - \frac{e}{c}N_{xx}\right). \tag{22}$$

It is worth emphasizing that the above equation accounts for stress assisted diffusion through N. The damage governing equation is given by

$$\dot{d} = \frac{1}{b} < \frac{E}{2}(\varepsilon - e\rho)^2 - < w(1-\lambda\rho) > + \kappa d_{xx} > . \tag{23}$$

By summarizing, and considering that $\varepsilon = u_x$, we have the following three balance equations to find the fields u, d and ρ:

$$\begin{cases} N = E(1-d)\left(u_x - e\rho\right), \\ \\ \dot{\rho} = D\left(\rho_{xx} - \dfrac{e}{c}N_{xx}\right), \\ \\ N_x + b = 0, \\ \\ \dot{d} = \dfrac{1}{b} < \dfrac{E}{2}(\varepsilon - e\rho)^2 - < w(1-\lambda\rho) > + \kappa d_{xx} > \end{cases} \tag{24}$$

together with appropriate boundary and initial conditions.

5. Numerical Aspects

In this section the computational model corresponding to the equations (24) is obtained as follows. First, the weak version of the mentioned equations are obtained. Then, temporal discretization is performed by using the backward Implicit Euler Method. The coupled system of equations so obtained are uncoupled by means of the operator splitting technic (staggered scheme). The spatial discretization is performed via the finite element method.

As already defined, let us consider a bar in a interval $[0, L]$, whose points are denoted by x, with the following essential boundary conditions: $u(0,t) = 0, \quad u(L,t) = u_L(t), \quad d(0,t) = d(L,t) = 0, \quad \rho(0,t) = \rho_0(t), \quad \rho(L,t) = \rho_L(t)$. We also assume that $b = 0$. Thus, we have the following weak form from equations (24):

Given : L, T, E, e, b, a, κ, c, M, $u_L(t)$, $\rho_0(t)$, $\rho_L(t)$

$$u(0,t) = 0, \quad u(L,t) = u_L(t), \quad d(0,t) = d(L,t) = 0, \quad \rho(0,t) = \rho_0(t), \quad \rho(L,t) = \rho_L(t),$$
$$u(x,0) = d(x,0) = \rho(x,0) = 0$$

$$\text{Find}: \{\rho, u, d\} : [0, L] \times [0, T] \mapsto \Re$$

$$\text{Such that}: \int_0^L \dot{\rho}\,\alpha\,\mathrm{dx} + \int_0^L D\rho_x\alpha_x\,\mathrm{dx} = 0 \quad \forall\ \alpha\ \in\ V^0,$$

$$\int_0^L (1-d)\ (u_x - e\rho)\,v_x\,\mathrm{dx} = 0 \quad \forall\ v\ \in\ V^0, \tag{25}$$

$$\int_0^L \frac{2b}{E}\,\dot{d}\,\gamma\,\mathrm{dx} + \int_0^L \kappa\,d_x\,\gamma_x\,\mathrm{dx} - \int_0^L (u_x - e\rho)^2\,\gamma\,\mathrm{dx} + \int_0^L a(\rho)\,\gamma\,\mathrm{dx} = 0 \quad \forall\ \gamma\ \in\ V^0,$$

where V^0 is the space of smooth functions $f(x)$ defined on $[0, L]$, so that $f(0) = f(L) = 0$.

A backward Euler scheme has been adopted for temporal discretization, thus we replace the time interval $[0, T]$ by the set $\mathcal{T} = \{t_0 = 0, t_1, ..., t_{k-1}, t_k, ...t_N = T\}$. Then the equations (25) become:

$$\begin{aligned} &a_\rho^k(\rho^k, \alpha) = l_\rho^k(\alpha),\\ &A_u^k(u^k, v; d^k) = L_u^k(v; d^k, \rho^k),\\ &a_d^k(d^k, \gamma) = L_d^k(\gamma; u^k, \rho^k), \end{aligned} \tag{26}$$

where

$$\begin{aligned} &a_\rho^k(\rho^k, \alpha) := \int_0^L \frac{\rho^k}{\Delta t}\alpha\,\mathrm{dx} + \int_0^L D\rho_x^k\alpha_x\,\mathrm{dx}, \qquad l_\rho^k(\alpha) := \int_0^L \frac{\rho^{k-1}}{\Delta t}\alpha\,\mathrm{dx},\\ &A_u^k(u^k, v; d^k) := \int_0^L (1-d^k)u_x^k v_x\mathrm{dx}, \qquad L_u^k(v; d^k, \rho^k) := \int_0^L E\,(1-d^k)\,\rho^k v_x\mathrm{dx},\\ &a_d^k(d^k, \gamma) := \int_0^L \frac{2\,b}{E\,\Delta t}d^k\gamma\,\mathrm{dx} + \int_0^L \kappa d_x^k\gamma_x\mathrm{dx},\\ &L_d^k(\gamma; u^k, \rho^k) := \int_0^L \frac{2\,b}{E\,\Delta t}d^{k-1}\gamma\,\mathrm{dx} + \int_0^L \left(u_x^k - e\,\rho^k\right)\gamma\,\mathrm{dx} - \int_0^L a(\rho^k)\,\gamma\,\mathrm{dx}, \end{aligned} \tag{27}$$

where the superscripts k and $k-1$ refer respectively to time instant t_k and t_{k-1}, while $\Delta\,t = t_k - t_{k-1}$ and $f^k = f(t_k)$.

The operator splitting method was used to solve the coupled equations system (26). In the present context this technique was used in the following sequence: at first ρ_k is calculated by using $(26)_1$, then u_k is calculated in $(26)_2$ by considering d^{k-1} and ρ_k obtained before, and finally d_k is obtained in $(26)_3$ by using u^k and ρ_k already obtained. Therefore, if we define:

$$\begin{aligned} &a_u^k(u^k, v) = A_u^k(u^k, v; d^{k-1}),\\ &l_u^k(v) = L_u^k(v; d^{k-1}, \rho^k),\\ &l_d^k(\gamma) = L_d^k(\gamma; u^k, \rho^k), \end{aligned} \tag{28}$$

the problem (26) can be rewritten:

$$\text{Given}: L,\ T,\ E,\ e,\ b,\ a,\ \kappa,\ c,\ M,\ N$$

$$\mathcal{T} = \{t_0 = 0, t_1, ..., t_{k-1}, t_k, ...t_N = T\}$$

$$u_L, \rho_L, \rho_0 : \mathcal{T} :\mapsto \Re$$

$$u(x, 0) = d(x, 0) = \rho(x, 0) = 0$$

$$\text{Find, for}\quad k = 1, N: \quad \{\rho, u, d\} : [0, L] \times [0, T] \mapsto \Re$$

$$\text{Such that, for}\quad k = 1, N: \quad a_\rho^k(\rho^k, \alpha) = l_\rho^k(\alpha), \quad \forall\ \alpha\ \in\ V^0,$$

$$a_u^k(u^k, v) = l_u^k(v), \quad \forall\ v\ \in\ V^0, \tag{29}$$

$$a_d^k(d^k, \gamma) = l_d^k(\gamma), \quad \forall\ \gamma\ \in\ V^0,$$

$$u(0,t_k)=0,\ u(L,t_k)=u_L(t_k),\ d(0,t_k)=d(L,t_k)=0,\ \rho(0,t_k)=\rho_0(t_k),\ \rho(L,t_k)=\rho_L(t_k).$$

Observe that a_ρ^k is bilinear in ρ_k, a_u^k is bilinear in u_k and a_d^k is bilinear in d_k, whereas l_ρ^k is linear in α, l_u^k is linear in v and l_d^k is linear in γ.

The spatial discretization is now described. Initially we write:

$$\rho^k=\rho_k+\bar{\rho}^k,\quad u^k=u_k+\bar{u}^k,\quad d^k=d_k+\bar{d}^k, \tag{30}$$

where u_k, d_k and ρ_k belong to V^0 whereas $\bar{u}^k$, $\bar{d}^k$ and $\bar{\rho}^k$ are known fuctions that obey the boundary conditions. We approach the space V^0 by the finite dimension space V^h, so that the functions $\bar{\rho}^k$, $\bar{u}^k$ and $\bar{d}^k$ belong to V^k.

Let $0=x_1<...<x_{nn}=L$ be a mesh of domain $\Omega=[0,L]$, where nn is the number of nodes and x_i is the coordinate of the node i. We define $\Omega_e=[x_e,x_{e+1}]$ the e-th element whose length is $h_e=x_{e+1}-x_e$. The index e varies from 1 to ne, where $ne=nn-1$ is the number of elements. In a uniform mesh, $h_e=h=\dfrac{L}{ne}$. We approach V^0 by the space V^h of the continuum and linear functions in each element. A generic element g from V^h can be written:

$$g(x)=\sum_{i=1}^{ne-1} g_i\Psi_i(x) \tag{31}$$

where the base functions Ψ_i, $i=1$, $ne-2$ are such that, for each i, $g(x_i)=g_i$, where g_i is the nodal value of g in the node i. It can be shown that:

$$\Psi_i(x)=\begin{cases}\dfrac{x-x_i}{h}, & x\in\Omega_i\\ \dfrac{x_{i+2}-x}{h}, & x\in\Omega_{i+1}\\ 0, & \text{otherwise.}\end{cases} \tag{32}$$

Thus, ρ_k, u_k, d_k, α, v and γ are approached as the generic function above, and the respective nodal values are stored in the vectors $\mathbf{p}_k$, $\mathbf{u}_k$, $\mathbf{d}_k$, $\mathbf{a}$, $\mathbf{v}$ and $\mathbf{g}$. The functions $\bar{\rho}^k$, $\bar{u}^k$ e $\bar{d}^k$ are chosen, respectively as:

$$\bar{\rho}^k=\rho_0(t_k)\Psi_0+\rho_L(t_k)\Psi_L,\quad \bar{u}^k=u_L(t_k)\Psi_L,\quad \bar{d}^k=0, \tag{33}$$

where:

$$\Psi_0(x)=\begin{cases}-\dfrac{x}{h}, & x\in\Omega_1\\ 0, & \text{otherwise.}\end{cases}\qquad \Psi_L(x)=\begin{cases}\dfrac{x-L}{h}, & x\in\Omega_{ne}\\ 0, & \text{otherwise.}\end{cases} \tag{34}$$

By substituting the above approximations in equation (29), we have:

$$\begin{aligned}&\mathbf{M}_k\mathbf{p}_k\cdot\mathbf{a}=\mathbf{G}_k\cdot\mathbf{a}\quad ,\forall\ \mathbf{a}\in\ \Re^{ne-1},\\ &\mathbf{K}_k\mathbf{u}_k\cdot\mathbf{v}=\mathbf{F}_k\cdot\mathbf{v}\quad ,\forall\ \mathbf{v}\in\ \Re^{ne-1},\\ &\mathbf{L}_k\mathbf{d}_k\cdot\mathbf{g}=\mathbf{H}_k\cdot\mathbf{g}\quad ,\forall\ \mathbf{g}\in\ \Re^{ne-1},\end{aligned} \tag{35}$$

where:

$$\begin{aligned}&(\mathbf{M}_k)_{ij}=a_\rho^k(\Psi_i,\Psi_j),\quad (\mathbf{G}_k)_i=l_\rho^k(\Psi_i)-\rho_0(t_k)a_\rho^k(\Psi_0,\Psi_i)-\rho_L(t_k)a_\rho^k(\Psi_L,\Psi_i),\\ &(\mathbf{K}_k)_{ij}=a_u^k(\Psi_i,\Psi_j),\quad (\mathbf{F}_k)_i=l_u^k(\Psi_i)-u_l(t_k)a_u^k(\Psi_L,\Psi_i),\\ &(\mathbf{L}_k)_{ij}=a_d^k(\Psi_i,\Psi_j),\quad (\mathbf{H}_k)_i=l_d^k(\Psi_i)-a_d^k(\Psi_0+\Psi_L,\Psi_i),\end{aligned} \tag{36}$$

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

The resulting algorithm is described as follows:

- Given: L, T, E, e, b, a, κ, c, M, ne, $u_l(t)$, $\rho_0(t)$, $\rho_L(t)$
- Initializations: $t_k=0$, $u(x,0)=d(x,0)=\rho(x,0)=0$, $k=1$
- For each time step, while $t_k\le T$
  - By calculating $\mathbf{M}_k$ and $\mathbf{G}_k$, obtain $\mathbf{p}_k$ by: $\mathbf{M}_k\mathbf{p}_k=\mathbf{G}_k$
  - By calculating $\mathbf{K}_k$ and $\mathbf{F}_k$, obtain $\mathbf{u}_k$ by: $\mathbf{K}_k\mathbf{u}_k=\mathbf{F}_k$
  - By calculating $\mathbf{L}_k$ and $\mathbf{H}_k$, obtain $\mathbf{d}_k$ by: $\mathbf{L}_k\mathbf{d}_k=\mathbf{H}_k$
  - Update: $k=k+1$ and return

6. Numerical Results

In this section we illustrate the application of the foregoing numerical model. We consider two situations corresponding to different constant values for the solute density: $\rho = 0$ and $\rho > 0$. The numerical parameters needed for the simulation were chosen just for illustrative purposes. Figure 1 and Figure 2 depict the damage and displacement distributions along the bar for a given time instant. Figure 3 depicts the graph $\epsilon \times N$ at the center of the bar. The deleterious effect of the solute can be clearly observed.

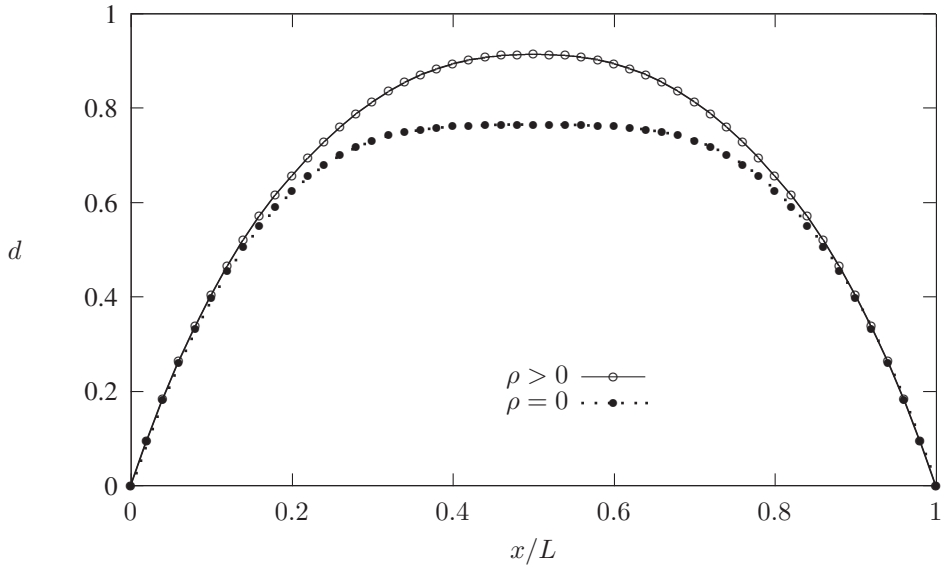

Figure 1. Damage distribution along the bar

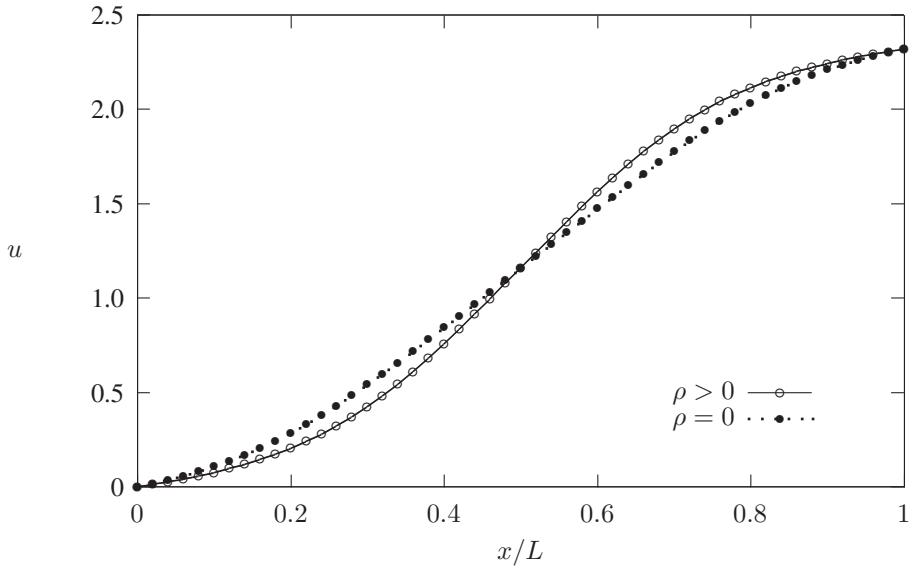

Figure 2. Displacement distribution along the bar

7. Conclusions

The aim of this work was the development of an one dimensional theory for linear elasticity coupled with damage and diffusion. In the theory, which was formulated within the framework of continuum mechanics, deformation-damage-diffusion coupling was implemented by way of the constitutive equations. A simplified version of the theory was obtained which served as the starting point for the development of a numerical model. The numerical model was based on the finite element method, the backward finite difference scheme and the operator splitting technique. An very naive example was

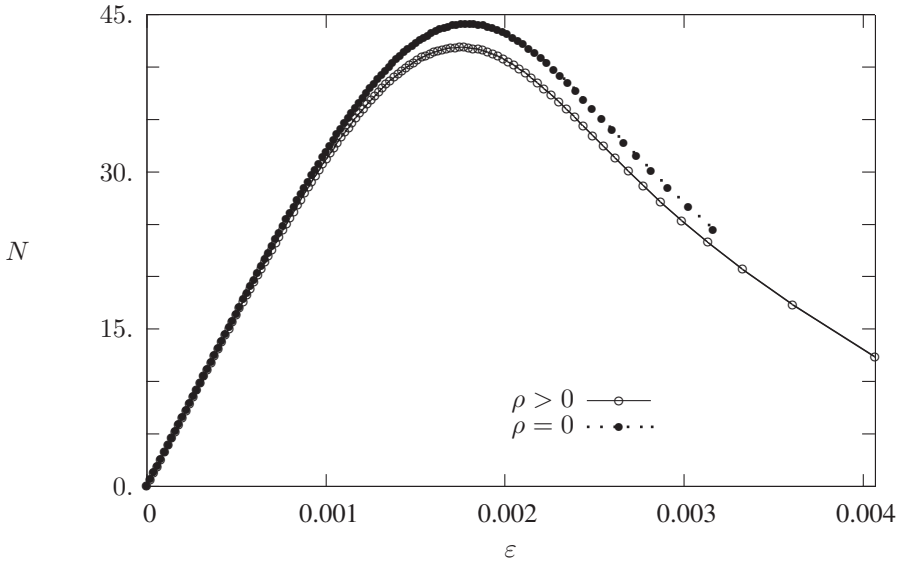

Figure 3. Stress-Strain curve at $x = L/2$

provided in order to illustrate the application of the numerical model.

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9. References

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