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A numerical study of a nonlocal model of damage propagation under chemical aggression

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We introduce a differential model to study damage accumulation processes in the presence of chemical reactions. The influence of micro-structure leads to a nonlinear parabolic system characterized by the presence of a characteristic length. Here, we first present an analytical description of the qualitative behaviour of solutions which blow-up in finite time. Numerical simulations are given to describe the shape of solutions near the rupture time and the influence of the chemical reagents. As in the non-reactive model, the failure of the material occurs in a region of positive measure, due to the diffusive effects of the micro-structure, although some localization phenomena are observed. Moreover, if we increase the chemical concentration beyond a given threshold, which depends upon the specific conditions of the material, we observe a strong acceleration in the damage process.

1 Introduction

In this paper, we consider a differential system, first proposed by Barenblatt [1], which describes the evolution of damage in a specimen of homogeneous material under the effect of mechanical stress and chemical aggression. Here we restrict our analysis to the isotropic one-dimensional case, where the damage is represented by a scalar function $0 \leqslant \omega \leqslant 1$, which can be considered as an averaged fraction of broken bonds inside a micro-structural element of the body. Therefore in the pristine material we have $\omega = 0$ everywhere, and $\omega = 1$ in the points of fracture. Damage theory, originally developed by Kachanov [9, 10, 11] (see also Odqvist & Hult [16]), is based on simple ordinary differential equations of the form

$$\dot{\omega} = \tau^{-1} q(\omega, \sigma), \tag{1.1}$$

that govern the damage evolution, where τ is a characteristic time and q is the damage accumulation rate. Despite its simplicity, this approach has been proven to be quite effective, and is still used by engineers as it provides a good agreement with experimental results. However, the behaviour of more complex materials (metals, ceramics, composites, etc.), as well as the imprecise knowledge of the stress tensor σ, was the main motivation of Barenblatt & Prostokishin [3] for replacing (at least in the one-dimensional case) the stress function σ by its weighted average. This led to a nonlinear parabolic equation, containing a micro-structural parameter λ, which depends upon the material and which can be interpreted as the characteristic interaction distance between different micro-grains of the specimen. The analytical investigations of Bertsch & Bisegna [5] demonstrated a perfect agreement with the numerical results of Barenblatt & Prostokishin [3].

Let us now briefly discuss some connections of our research with existing engineering investigations. Although there is now a huge and well established community working on damage problems, it is very difficult to find a single, universally accepted model, even if there is now general agreement about the non-local nature of damage (see also, for instance, Pijaudier-Cabot & Bazant [17] and Bazant [4]). Moreover, even its experimental evaluation is a matter of investigation, since it is difficult to give a general and direct procedure for damage measurement. There are also a few models which take into account the interaction between damage and chemistry, but it is hard to find rigorous works in this direction. Some experimental works, and even modelling, have been done for particular problems in civil engineering [12, 13], for damage of concrete under aggressive water attack, for alkali-aggregate reactions [6, 7, 14], but it is still a completely non-trivial task to relate these simulations and observations to precise mathematical statements. In conclusion, the mathematical damage theory under chemical aggression is not yet a fully developed field, and mathematical and numerical work still has to be done to extract more information from the models, and to create a clear set of predictions to be evaluated in the tests.

In this context, the main goal of the present paper is investigation of a new one-dimensional model that also takes into account aggression by chemical reagents. The model consists of a system of strongly-coupled nonlinear parabolic equations. In § 2 we present both models (reactive and non-reactive) and some existence results, as well as the blow-up properties of the solutions; in § 3 we approximate these solutions by a semi-implicit scheme. We discuss some numerical tests, pointing out the differences and the analogies between the two models, with and without chemical aggression. We point out that the numerical investigation is particularly significant in relation to the pure analytical one, since we can detect and investigate new qualitative phenomena, which for the moment are not predicted by the theory.

The main result of our analysis is that the geometry of the damage front is not essentially influenced by chemical aggression, but we have a strong acceleration of the damage evolution. According to our numerical tests, we observe (§ 4.2) that the damage diffusion is rather negatively influenced by the chemical action, due to a clear localization mechanism. This fact is qualitatively in agreement with the results of Le Bellego *et al.* [12, 13], and is due to the modification in time of the internal characteristic length, namely our micro-structural parameter λ. We observe also that, if we increase the given concentration of chemical reagents beyond a threshold, the rupture time dramatically decreases. In conclusion, we expect that, if applied to more realistic models, this kind of behaviour should be relevant for monitoring the damage evolution in materials exposed to external pollution and to fix the critical levels of attention.

2 Nonlocal damage models

2.1 The basic model

We consider a prismatic specimen with a cross-section of area Ω_0 to which a constant load F is applied in the x direction. We denote by $\Omega(x)$ the area of the cross-section able to support the load at point x. In each cross-section, there are parts that are pristine and parts that, due to imperfections or cracks, are no more able to sustain the load. Following Kachanov [11], we define the damage factor

$$\omega(x) = \frac{\Omega_0 - \Omega(x)}{\Omega_0}.$$

We consider the nominal stress $\sigma_0 = \frac{F}{\Omega_0}$ generated by a load F, which is parallel to the axis of the specimen, and we define the actual stress $\sigma(x)$ in a specific cross-section x as

$$\sigma = \frac{F}{\Omega(x)}. \tag{2.1}$$

Therefore, a relation between the actual stress and the damage is obtained:

$$\sigma = \frac{\sigma_0}{1-\omega}. \tag{2.2}$$

We assume now that the damage evolution is governed by a kinetic equation of the type (see Kachanov [11])

$$\dot{\omega} = \tau^{-1} q(\omega, \sigma). \tag{2.3}$$

Here τ represents the characteristic time of the process and q is a dimensionless non-negative function which depends upon the material. Typical expressions for q are [3]:

- Arrhenius type:

  $$q(\omega, \sigma) = (1-\omega)^p e^{-\frac{U-\gamma\sigma}{kT_0}}, \tag{2.4}$$

  where k is the Boltzmann constant, $U > 0$ the activation energy, $\gamma > 0$ is the rate of the activation-energy with respect to the stress, and p is the order of the reaction and T_0 is the temperature.

- Power type:

  $$q(\omega, \sigma) = C(1-\omega)^p \left(\frac{\sigma}{\sigma_0}\right)^n,$$

  n is a constant, C depends upon the temperature, and p, as before, is the order of the reaction.

The rupture time of the specimen is defined as the first time at which ω is equal to 1 in some point.

Equation (2.3) is well known in mechanics, and often arises in applications (see Kachanov [11]). However, for complex materials, this model is no longer realistic. For example, given a non-homogeneous initial distribution of damage, this model trivially implies that the specimen will break at the points of maximum initial damage, and the rupture time will depend only on the magnitude of this maximum, but not on the value of ω in the neighbouring cross-section.

In Barenblatt & Prostokishin [3], the authors proposed to replace (2.3) by a new equation, which takes into account non-local effects. The main point is the fact that the damage accumulation rate in a cross-section is supposed to depend also on the damage and on the stress at neighbouring cross-sections. Let ρ be a weight function which is related to the micro-structural properties of the material, by taking into account the long distance interactions bewtween molecules. Assume that ρ is rapidly decaying at infinity, but possibly with a compact support, and satisfies

$$\int_{-\infty}^{+\infty} \rho(x)\,dx = 1, \quad \int_{-\infty}^{+\infty} x\rho(x)\,dx = 0. \tag{2.5}$$

We replace the kinetic equation (2.3) by a new one, where we make a convolution of the original kinetic function q, with ρ. This yields a kinetic integro-differential equation

$$\partial_t \omega = \tau^{-1} \int_{-\infty}^{+\infty} \rho(\xi) q(\omega(x-\xi),\, \sigma(x-\xi))\,d\xi. \tag{2.6}$$

We are tacitly assuming that the function ρ is so concentrated that integral limits can be taken at infinity. In principle, this function ρ could exist, but it is unfortunately difficult to recover from the material properties. In general, in all the nonlocal approaches (see, for instance, Plaudier-Cabot & Bazant [17], a Gaussian kernel is given with only one free parameter, Furthermore, we can formally approximate q by its second order Taylor expansion

$$\begin{aligned} q(\omega(x-\xi), \sigma(x-\xi)) \approx{}& q(\omega(x), \sigma(x)) + \partial_x q(\omega(x), \sigma(x))\xi \\ &+ \partial_{xx} q(\omega(x), \sigma(x)) \frac{\xi^2}{2}. \end{aligned}$$

Let us set

$$\lambda^2 := \int_{-\infty}^{+\infty} \frac{x^2}{2} \rho(x)\,dx. \tag{2.7}$$

If we replace the Taylor expansion in (2.6), we obtain a partial differential equation

$$\partial_t \omega = \tau^{-1} [q(\omega, \sigma) + \lambda^2 \partial_{xx} q(\omega, \sigma)]_+. \tag{2.8}$$

Here the damage process is no longer depending on the special form of the weight function ρ, as in (2.6), but just depends upon the so called micro-structural length parameter λ. Notice that here we have taken the positive part on the right-hand side of (2.8), to avoid a non-physical regression of the damage. This is not required for (2.3) and (2.6), where non-negative initial data yield a non-negative time derivative.

It is worth comparing this approximation with respect to the original one. The first remark is the fact that the analytical and numerical theory of equations like (2.6) is not yet fully developed, and therefore the differential approach yields more information. Moreover, numerical tests reveal that, at least as long as the solution stays smooth, the solution of the differential approximation follows very closely the one given by the integral approach. Anyway, it is clear that further analytical investigations should be performed to keep or reject this kind of expansion.

Assuming now a finite length L of the bar, the natural boundary conditions that complete the problem are of Neumann type

$$\partial_x \omega(0,\cdot) = \partial_x \omega(L,\cdot) = 0.$$

Finally, substituting (2.2) into the expression of q, we set

$$Q(\omega) = q\left(\omega, \frac{\sigma_0}{1-\omega}\right). \tag{2.9}$$

Then, and rewriting the system for the new variable, we obtain

$$\begin{cases} \partial_t \omega = \tau^{-1}[Q(\omega) + \lambda^2 \partial_{xx} Q(\omega)]_+, \\ \partial_x \omega(0,t) = \partial_x \omega(L,t) = 0. \end{cases} \tag{2.10}$$

Equation (2.10) was studied in detail in Bertsch & Bisegna [5], where existence results and some properties of the solution were established.

2.2 Damage under chemical aggression

In this section, we present a model which has first been proposed by Barenblatt [1]. Again, we consider a one-dimensional symmetry, for example a prismatic specimen of homogeneous material, but in this case we suppose that a chemical reagent is penetrating in the block. Following the Kachanov approach [11] again, we assume that, if $c(x,t)$ is the concentration of reagent in the cross-section x at time t, equation (2.3) takes the form

$$\dot{\omega} = \tau^{-1}\mathscr{B}(c)q(\omega,\sigma), \tag{2.11}$$

where $\mathscr{B}(c)$ is a non-decreasing function such that $\mathscr{B}(0) = 1$, and q is defined as above.

By arguing as in the case without chemistry, we can obtain from (2.11) a system of differential equations that describes the behaviour of damage in presence of chemical reagent. Under the standard Fick law [2], we can suppose that the reagent concentration c satisfies a nonlinear diffusion equation

$$\partial_t c = \partial_x(D(\omega)\partial_x c) + r(x,t,c), \tag{2.12}$$

where $r(x,t,c)$ is a source term, which takes into account the dissipation of the chemical reactant, D is a smooth non-negative function, with $D' \geqslant 0$. For the sake of simplicity, in the following we take the function $r(x,t,c) \equiv 0$.

If now, as in the previous section, we introduce a non-local dependence of damage and stress on the neighbouring cross-sections, it is natural to make a convolution between (2.11) and a weight function ρ,

$$\partial_t \omega = \tau^{-1} \int_{-\infty}^{+\infty} \rho(x-\xi)\mathscr{B}(c(x))q(\omega(\xi),\sigma(\xi))\,d\xi. \tag{2.13}$$

By making the Taylor expansion, we obtain

$$\partial_t \omega = \tau^{-1}\mathscr{B}(c)[Q(\omega) + \lambda^2 \partial_{xx} Q(\omega)]_+, \tag{2.14}$$

where Q is defined as in (2.9). Finally, coupling (2.14) and (2.12), the following system arises:

$$\begin{cases} \partial_t\omega = \tau^{-1}\mathscr{B}(c)[Q(\omega) + \lambda^2\partial_{xx}Q(\omega)]_+, \\ \partial_t c = \partial_x(D(\omega)\partial_x c), \\ \partial_x\omega(0,t) = \partial_x\omega(L,t) = 0, \\ c(0,t) = c_l \text{ and } c(L,t) = c_r, \end{cases} \tag{2.15}$$

where the two constants c_r and c_l are our boundary data. Here, as previously, the positive part is taken to keep the solution increasing in time.

Remark 2.1 It is worth noticing that, instead of (2.13), several choices are possible; for instance we could assume that the damage accumulation rate depends upon the damage $q(\omega, \sigma, c)$, the stress and the concentration of reagent of neighboring cross-section and this would lead to

$$\partial_t\omega = \tau^{-1}\int_{-\infty}^{+\infty} \rho(x-\xi)\mathscr{B}(c(\xi))q(\omega(\xi),\sigma(\xi))\,d\xi. \tag{2.16}$$

Now, again expanding (2.16) up to the second order terms gives

$$\partial_t\omega = \tau^{-1}[\lambda^2\partial_{xx}(\mathscr{B}(c)Q(\omega)) + \mathscr{B}(c)Q(\omega)]_+.$$

However, the presence of second derivatives of c in the kinetic equation is actually unrealistic. Take, for instance, an initial concentration of the reagent which is highly oscillating. Numerical experiments show unrealistic behaviour, since the blow-up times are shorter for these initial data than for those obtained with a saturated concentration of the reagent.

2.3 Analytical backgrounds: existence results and blow-up properties of solutions

We recall here some recent analytical results about system (2.15), which have been proven in Nitsch [15]. First, let us rewrite the system in a more convenient form. Multiplying the first equation in (2.15) by $Q'(\omega)$, and setting $u \equiv Q(\omega(x,t))$, $g(\cdot) \equiv \tau^{-1}Q'(Q^{-1}(\cdot))$, $G(u) \equiv D(\omega(u))$, we obtain

$$\begin{cases} \partial_t u = \mathscr{B}(c)g(u)[u + \lambda^2\partial_{xx}u]_+, \\ \partial_t c = \partial_x(G(u)\partial_x c), \\ \partial_x u(0,t) = \partial_x u(L,t) = 0, \\ c(0,t) = c_l, \ \ c(L,t) = c_r. \end{cases} \tag{2.17}$$

where, setting $\mu = Q(0)$, $u \geqslant \mu > 0$, and $g(u)$ is a smooth function with a super-linear growth. Obviously, the state $u = \mu$ corresponds to $\omega = 0$ and there is no damage, while $\omega = 1$ (rupture), corresponds to $u = +\infty$. So the study of the creeping process is rewritten as a blow-up problem.

Since we are dealing with a fully nonlinear degenerate parabolic system, we do not expect global existence of classical solutions. Therefore, we need to deal with a weaker form of solutions. From now, we assume $G \in C^{\infty}$, and, without loss of generality, $L = 1$.

Definition 2.2 *A couple* $(u, c) : [0,1] \times [0,T] \to [\mu, +\infty) \times [0,1]$ *is a solution of the problem* (2.17) *for the initial conditions* (u_0, c_0) *if for some* $0 < \alpha < 1$*:*

- $u \in C^{1,1}([0,1] \times [0,T))$, $c \in C^{2+\alpha, 1+\alpha/2}([0,1] \times [0,T))$, *and* u_x *is Lipschitz continuous in* $[0,1]$, *uniformly with respect to* t *in compact subset of* $[0,T)$*;*
- $u(0,t) = u(1,t) = 0$, *for all* $t \in [0,T)$*;*
- $u(x,0) = u_0(x)$, *and* $c(x,0) = c_0(x)$, *for all* $x \in [0,1]$*;*
- $\partial_t u = \mathscr{B}(c) g(u)[u + \lambda^2 \partial_{xx} u]_+$ *for* $t \in (0,T)$ *and a. e. in* $(0,1)$*;*
- $\partial_t c = \partial_x (G(u) \partial_x c)$. *for all* $(t,x) \in (0,1) \times (0,T)$*;*

Theorem 2.3 [15] *Let* $u_0(x) \in C^1[0,1]$, *with* $u_0 \geqslant \mu$, *and* $c_0(x) \in C^{2+\alpha}[0,1]$ *with* $0 < \alpha < 1$, *which satisfy the boundary conditions*

$$\begin{aligned} &\partial_x u_0(0) = \partial_x u_0(1) = 0, \\ &c_0(0) = c_l, \;\; c_0(1) = c_r; \end{aligned}$$

assume that the function u_0' *is Lipschitz continuous in* $[0,1]$ *, and there exists* $\Psi \in C([0,1])$ *such that* $u_0 \in C^2(\{\Psi > 0\})$ *and* $(\lambda^2 u_0'' + u_0)_+$ *a.e. in* $[0,1]$. *Then there exists a unique* (u,c) *and* $T < +\infty$, *such that* (u,c) *is solution to system* (2.17) *in* $[0,1] \times [0,T)$, *and*

$$\lim_{t \to T} \max_{0 \leqslant x \leqslant 1} u(x,t) = +\infty \qquad \text{as } t \to T.$$

The next result establishes a non-trivial property of the blow-up set for a special class of initial data.

Theorem 2.4 [15] *In the same hypotheses of Theorem 2.3, let* (u,c) *be a solution of* (2.17) *and* T *its blow-up time. Suppose that* $u_{0x} \leqslant 0$ *and* $c_{0x} \leqslant 0$. *Then there exists* β *such that*

$$B := \left\{ x \in [0,1] : \lim_{t \to T} u(x) = +\infty \right\} = [0, \beta],$$

where

$$B_- \equiv \min \left\{ \frac{\lambda \pi}{2}, 1 \right\} \leqslant \beta \leqslant \min \{ \lambda \pi, 1 \} \equiv B_+.$$

Roughly speaking, if u_0 and c_0 are monotone non-increasing functions, then the blow-up set of u has non zero measure, and a lower and upper bounds for its measure are given only in terms of the micro-structural parameter λ. We observe that, if $c \equiv 0$, the system reduces to (2.10), and we recover the results of Bertsch & Bisegna [5, Theorems 1.1, 1.2].

3 The numerical approximation

3.1 The case without chemical action

First, we discuss numerical solutions obtained for (2.10). A similar analysis was already performed in Barenblatt & Prostokishin [3], but here we reconsider those results, mainly to compare with the reactive case. Let us describe our numerical scheme. From now on, we only consider q of Arrhenius type, i.e. given by (2.4). It is also useful to introduce a simplification by a time scaling in (2.10), which now reads

$$\partial_\theta \omega = \left[(1-\omega)^p e^{\frac{\eta}{1-\omega}} + \lambda^2 \partial_{xx}\left((1-\omega)^p e^{\frac{\eta}{1-\omega}}\right)\right]_+, \tag{3.1}$$

where $M = \tau^{-1} e^{-\frac{U}{kT_0}}$, $\eta = \frac{\sigma_0 \gamma}{kT_0}$, and $\theta = Mt$ is the scaled time. It is also assumed that $L = 1$, without loss of generality. As usual, the solution is approximated by means of a sequence ω_j, which approaches ω at a grid point $x_j = j\Delta x$; here Δx is the space and scaled time steps. We also set $U_j \equiv Q(\omega_j) = (1-\omega_j)^p \exp(\frac{\eta}{1-\omega_j})$. After several numerical experiments, the more stable and efficient is the second order Runge–Kutta method applied to the system of ODE given by the space discretization (method of lines):

$$\dot{\omega}_j = \left\{\lambda^2 \frac{U_{j+1} - 2U_j + U_{j-1}}{\Delta x^2} + U_j\right\}_+. \tag{3.2}$$

This method is a parabolic version of the second order SSP-scheme of Gottlieb *et al.* [8]. The (formal) CFL condition gives the following space-dependent condition on $\Delta\theta$ (time step):

$$\Delta\theta \leqslant \frac{\Delta x^2}{2\lambda^2 \max_j Q'(\omega_j)}, \tag{3.3}$$

which is the same condition used for a scheme forward in time and central in space. Notice that in the following we only consider the time step given by the equality in formula (3.3). To give a numerical justification of this condition, we performed some numerical tests. Fix $\lambda = 0.1$, $\eta = 10$, $p = 1$ and take an initial datum which is small and well localized near the origin, namely

$$\omega_0(x) = 0.05 \exp(-20x). \tag{3.4}$$

We considered a time $T^* = 1$, which is greater than the half of the estimated blow-up time and we computed the solution at T^* for several different spatial meshes. The times are calculated in θ_0 units, where θ_0 is the rupture time obtained for the same initial condition, but evolving according to the ordinary differential equation (2.3). Notice that we cannot reach the blow-up time, since the scheme becomes unstable. However, we observe that the damage grows very rapidly beyond the value 0.4, and actually the time $\bar{T}$ at which the damage reaches this value is very close to the blow-up time. The results are presented in Table 1. In the first column there is the space step, in the central one the L^∞ error between the 'exact' solution (actually, just a fine approximation, using very small steps) and the approximated one, and in the last column we give the estimated order of accuracy. Here

Table 1. *The L^∞ errors in function of the space step, δ is the order of accuracy*

Δx	L^∞ error	δ
1/25	$7.6 \cdot 10^{-3}$	2.2
1/50	$1.7 \cdot 10^{-3}$	2.1
1/100	$3.9 \cdot 10^{-4}$	2.3
1/200	$7.8 \cdot 10^{-5}$	2.3

Table 2. *The estimated rupture time in function of the space step*

Δx	$\bar{T}_{\Delta x}$	$\bar{T}_{\frac{\Delta x}{2}} - \bar{T}_{\Delta x}$
1/25	1.6001	$3.7 \cdot 10^{-3}$
1/50	1.59644	$6.6 \cdot 10^{-4}$
1/100	1.59578	$1.4 \cdot 10^{-4}$
1/200	1.59564	$3.6 \cdot 10^{-5}$
1/400	1.5956	

and in the following, the numerical order of accuracy δ is given by the standard formula

$$\delta = \log_2 \left(\frac{e(h)}{e(h/2)} \right),$$

where $e(h)$ is the L^∞ error with a space step h.

We also investigated the behaviour of the estimated rupture time in function of the space step, see Table 2. In particular, in a good scheme the rupture time has to be independent of Δx, as $\Delta x \to 0$. We computed, for different space steps, the time $\overline{T}_{\Delta x}$ at which the damage first reaches the value 0.4 at some point, actually at $x = 0$. Table 2 shows a good stability of the numerical rupture time for $\Delta x \to 0$. We also observe that

$$\varepsilon_{\Delta x} \equiv T_{\frac{\Delta x}{2}} - T_{\Delta x} \approx \frac{T_{\Delta x} - T_{2\Delta x}}{4} \equiv \varepsilon_{2\Delta x}.$$

This means that, denoting by $T := \lim_{\Delta x \to 0} T_{\Delta x}$ the limit of the rupture times, we can estimate the error in the computation by the extrapolation formula

$$T - T_{\Delta x} \approx \varepsilon_{\Delta x} \sum_{n=0}^{+\infty} \left(\frac{1}{4} \right)^n = \frac{4}{3} \varepsilon_{\Delta x}.$$

This result is in perfect agreement with the RK numerical scheme second order accurate in time.

3.2 The case with chemical action

Here we restrict again our analysis to Arrhenius type damage accumulation rate, and in analogy with § 3.1, we perform a time-scaling on (2.15). This gives

$$\begin{cases} \partial_\theta \omega = \mathscr{B}(c)\left[(1-\omega)^p e^{\frac{\eta}{1-\omega}} + \lambda^2 \partial_{xx}\left((1-\omega)^p e^{\frac{\eta}{1-\omega}}\right)\right]_+, \\ \partial_\theta c = \partial_x(D(\omega)\partial_x c), \\ \partial_x u(0,t) = \partial_x u(L,t) = 0, \\ c(0,t) = c_l \text{ and } c(L,t) = c_r. \end{cases} \tag{3.5}$$

Our strategy is to implement a scheme that decouples the two differential equations of the system (3.5) The first equation in (3.5) has been approximated by an explicit scheme central in space and Runge–Kutta (second order) in time. As before, we also set $U_j \equiv Q(\omega_j) = (1-\omega_j)^p \exp(\frac{\eta}{1-\omega_j})$, to give

$$\dot{\omega}_j = \mathscr{B}(c_j)\left\{\lambda^2 \frac{U_{j+1} - 2U_j + U_{j-1}}{\Delta x^2} + U_j\right\}_+, \tag{3.6}$$

where we consider c_j constant during a time step. Once ω_j^{n+1} is computed from ω_j^n, the second equation, which is linear in c, is approximated by means of the standard Crank–Nicholson method

$$\frac{c_j^{n+1} - c_j^n}{\Delta\theta} = \tfrac{1}{2}\left\{D\left(\omega_j^n\right)\frac{c_{j+1}^n - 2c_j^n + c_{j-1}^n}{\Delta x^2} + \frac{D(\omega_{j+1}^n) - D(\omega_{j-1}^n)}{2\Delta x}\frac{c_{j+1}^n - c_{j-1}^n}{2\Delta x}\right\}$$

$$+ \tfrac{1}{2}\left\{D\left(\omega_j^{n+1}\right)\frac{c_{j+1}^{n+1} - 2c_j^{n+1} + c_{j-1}^{n+1}}{\Delta x^2} + \frac{D(\omega_{j+1}^{n+1}) - D(\omega_{j-1}^{n+1})}{2\Delta x}\frac{c_{j+1}^{n+1} - c_{j-1}^{n+1}}{2\Delta x}\right\}. \tag{3.7}$$

We used a semi-implicit two steps algorithm to compute the values of ω^{n+1} and c^{n+1} from ω^n and c^n. First, we obtain the value of ω^{n+1} from (3.6). Then c^{n+1} is obtained as the solution of the algebraic linear tridiagonal system arising from (3.7). The CFL condition is adapted in time to the size of the solution, and reads

$$\Delta\theta_n = \frac{\Delta x^2}{2\lambda^2 \max_j^n\{\max\{Q'\left(\omega_j^n\right), D\left(\omega_j^n\right)\}\}}.$$

To give a numerical justification of this condition, we performed some numerical tests.

Let us fix $\lambda = 0.1$, $p = 1$, $\eta = 10$, $D(\omega) = 10^4(1-\omega)^{-3}$, $\mathscr{B}(c) = 1 + (10c)^3$, $c_l = 0.2$, $c_r = 0$ and take the initial condition for ω given by (3.4). We considered a time $T^* = 0.5$ greater than the half of the blow-up time and we computed the solution at T^* for several different space steps. The results are reported in Table 3. In the first column there is the space step, in the central one the L^∞ error, between the 'exact' solution (actually just a fine approximation, using very small steps) and the approximated one, and in the last one the estimated order of accuracy. We also investigated the behaviour of the estimated rupture time in function of the space step. As for the case without the reacting term, we computed, for different space steps, the time $T_{\Delta x}$ at which the damage reaches the value 0.3 at some point. Again, the times are computed in θ_0 units, where θ_0 is the rupture time obtained for the same initial condition evolving accordingly to the ordinary differential

Table 3. *The L^∞ errors in function of the space step, δ represent the order of accuracy*

Δx	L^∞ error	δ
1/25	$2.7 \cdot 10^{-3}$	1.96
1/50	$7 \cdot 10^{-4}$	2.46
1/100	$1.3 \cdot 10^{-4}$	2.7
1/200	$2 \cdot 10^{-5}$	

Table 4. *The estimated rupture time in function of the space step*

Δx	$T_{\Delta x}$	$T_{\frac{\Delta x}{2}} - T_{\Delta x}$
1/25	0.7094	$1.1 \cdot 10^{-3}$
1/50	0.71052	$2.5 \cdot 10^{-4}$
1/100	0.71077	$1.5 \cdot 10^{-4}$
1/200	0.71092	$3.3 \cdot 10^{-4}$
1/400	0.71125	

equation (2.3). The numerical results are presented in Table 4 and show a general good behaviour of our scheme, even with respect to the blow-up time.

4 Computational results

4.1 The non-reacting case

In this last section, we shall use our scheme to investigate the qualitative properties of the solutions. The initial distribution of damage ω_0 is still given by (3.4). We present several simulations computed at different values of the micro-structural parameter λ. We used 200 nodes in space, and fixed $\eta = 10$ and $p = 1$. In the figures we consider the ratio θ/θ_0, where θ_0 is the rupture time obtained for the same initial condition, but evolving according to equation (2.3). Figures 1–3 represent the damage evolution for three different values of the micro-structural parameter $\lambda = 0.02, 0.1, 0.5$, respectively. In Figure 1, the damage remains concentrated near the origin; in Figure 2, the damage diffusion is sensible, but still contained in the interval $[0, 1]$ (the bar length); finally, in Figure 3 the damage spreads along all the bar length, and rapidly becomes flat. However, in all these numerical experiments, the blow-up set is well estimated by the theoretical bound given by Theorem 2.4, and the ratio θ/θ_0 near the rupture time is always greater than 1 for all λ, as a trivial consequence of the comparison principle. Unfortunately, a sharp estimate of the dependence of θ/θ_0 as a function of λ is still an open problem.

A first interesting consequence of the nonlocal model is that in the evolution process we can recognize two phases. In the first one, the 'pure diffusion phase', the maximum of ω does not change; this fact is peculiar to this kind of nonlocal models (see Barenblatt & Prostokishin [3]). A second phase is characterized by a rapid growth of ω. In Figure 4, we can see four curves, one standing for the initial datum ω_0, the others for the damage ω, for three different values of λ, all at the end of the 'pure diffusion phase', i.e. when

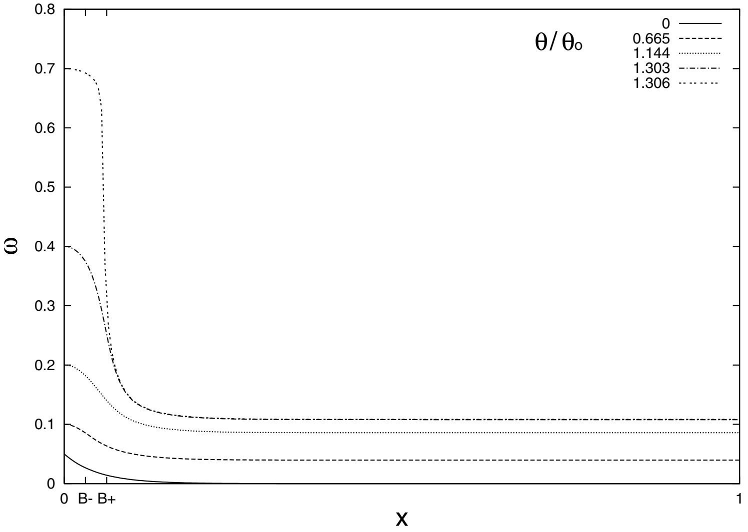

FIGURE 1. The evolution of damage ω with $\lambda = 0.02$.

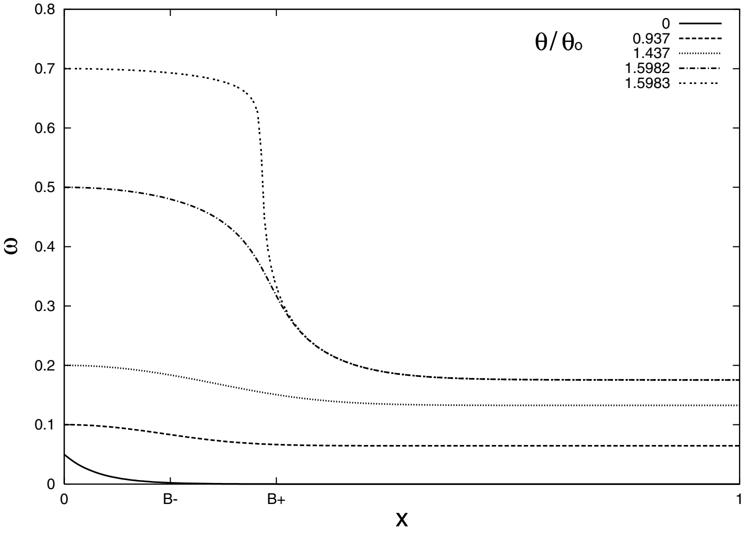

FIGURE 2. The evolution of damage ω with $\lambda = 0.1$.

the maximum value starts to grow. We observe that, as expected, the diffusion is bigger for larger values of λ. Moreover, by comparing time intervals in Figure 4 with those in Figures 1–3, the time spent during the 'pure diffusion' evolution increases with λ.

4.2 The reacting case

We investigated now the behaviour of the solutions of the problem (3.5). Let us fix, as in § 3, $p = 1$, $\eta = 10$, $D(\omega) = 10^4(1-\omega)^{-3}$, $\mathscr{B}(c) = 1+(10c)^3$. In Figures 5–7 we present some

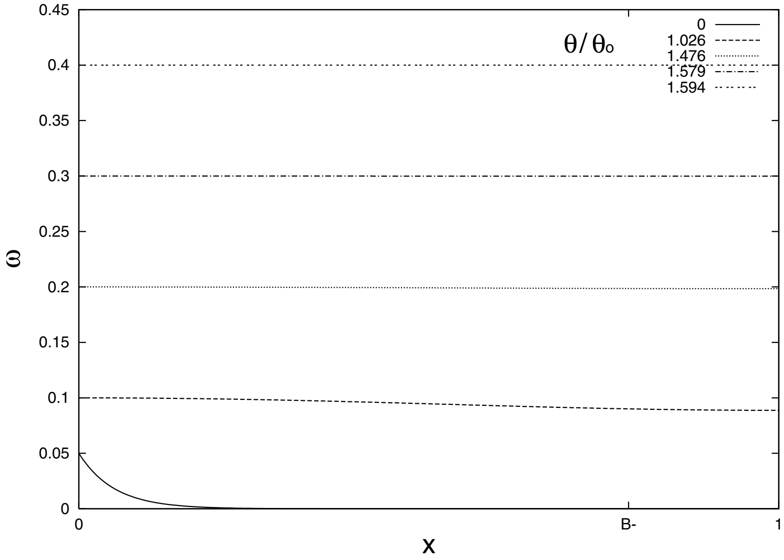

FIGURE 3. The evolution of damage ω with $\lambda = 0.5$.

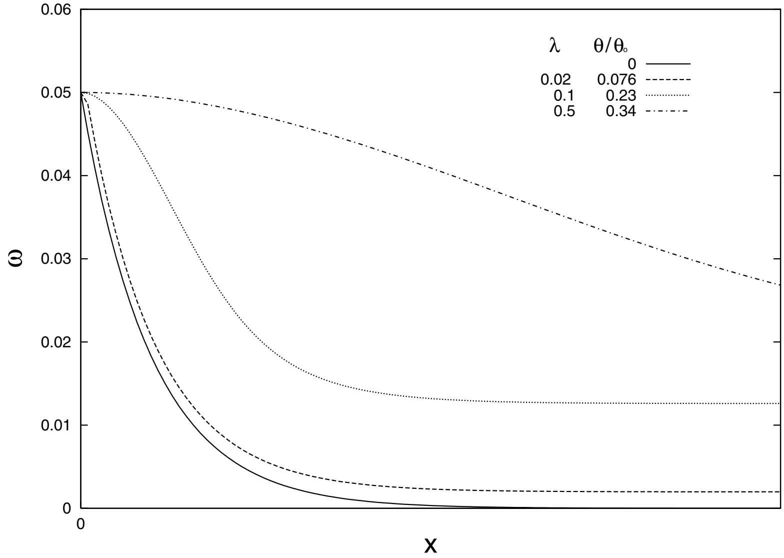

FIGURE 4. The damage evolution at the end of the pure diffusion process, for three different values of λ, compared with the initial datum ω_0.

simulations with 200 space nodes and $\lambda = 0.02$, 0.1, 0.5, respectively. The initial damage ω_0 is the same used in the case without the chemical interaction, namely it is given by 3.4. The initial density of the reagent is concentrated at $x = 0$

$$c_0(x) = c_l \exp(-30x)$$

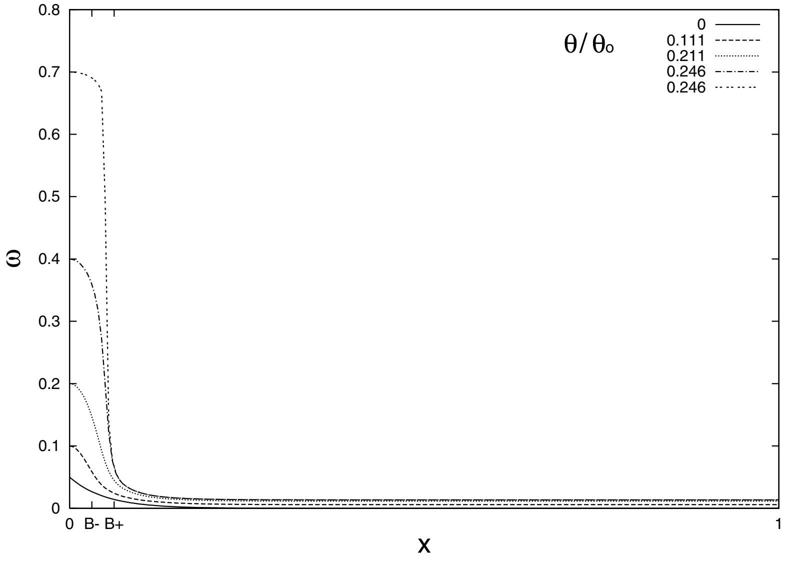

FIGURE 5. The evolution of damage ω with $\lambda = 0.02$.

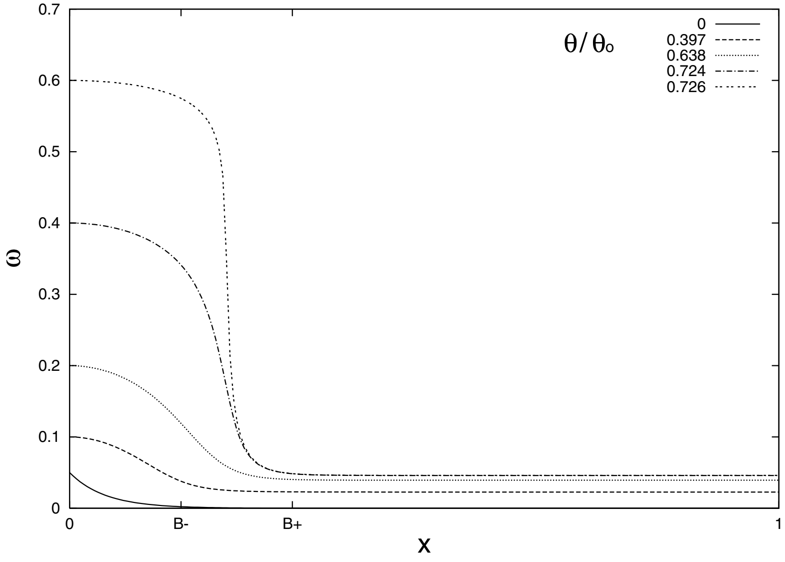

FIGURE 6. The evolution of damage ω with $\lambda = 0.1$.

and the boundary conditions are $c_r = 0$ and $c_l = 0.2$. Again, we label the curves by the dimensionless ratio θ/θ_0.

First let us observe that, because of the chemical aggression, the rupture times are now shorter. Again, we observe the different behaviour of the specimen, according to the different values of λ. Figure 5 is similar to Figure 1, with a small damage diffusion along the specimen, while in Figures 6 and 7, the damage diffusion clearly increases compared

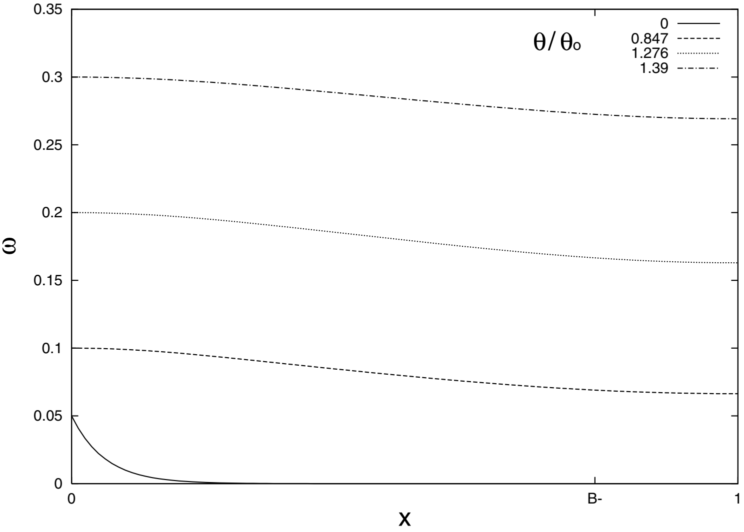

FIGURE 7. The evolution of damage ω with $\lambda = 0.5$.

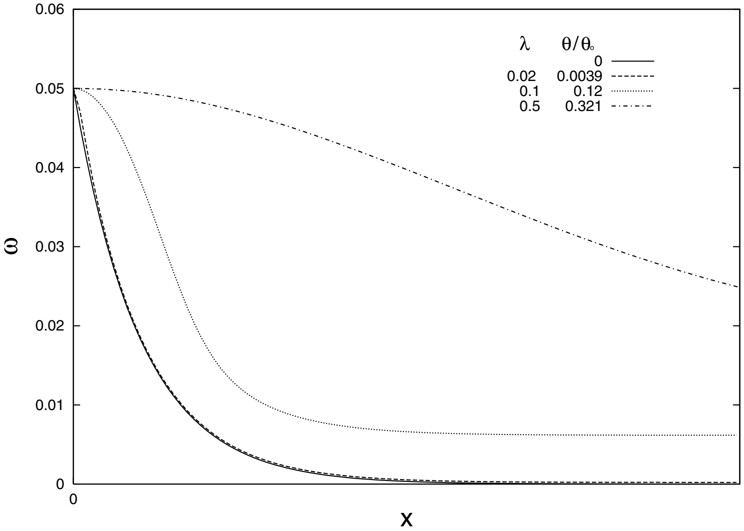

FIGURE 8. The damage evolution at the end of the pure diffusion process (with chemistry), for three different values of λ, compared with the initial datum ω_0.

to Figure 5, but it shows a sort of localization with respect to the non-reactive case. In particular, in Figure 7 the damage spreads out along all the specimen, but the chemistry prevents ω from becoming as flat as in Figure 3. Finally, notice that in all these examples, the blow-up sets are smaller than those in Figures 1–3, even though obviously they still satisfy the bounds given in Theorem 2.4.

Table 5. *The (estimated) rupture time for different value of boundary concentration of λ over the (estimated) rupture time in absence of microstructure ($\lambda = 0$)*

c_l	$T_{\lambda=0.1}/T_{\lambda=0}$	$T_{\lambda=0.02}/T_{\lambda=0}$
0	1.6	1.3
0.5	35	3.8
0.9	125	5.2

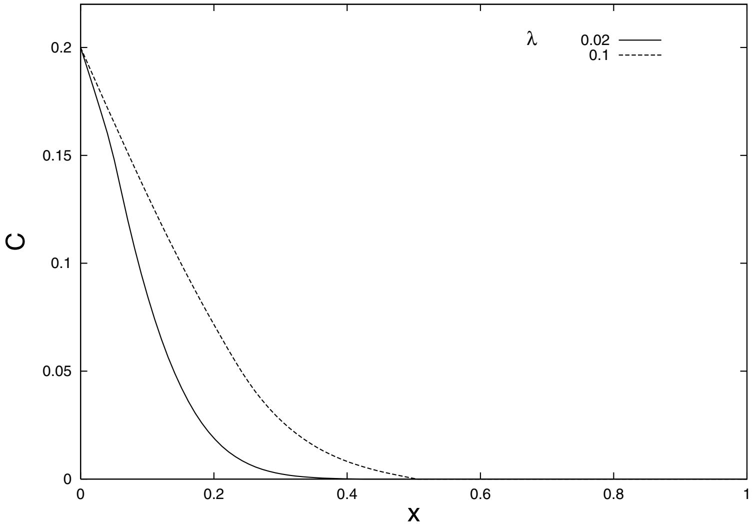

Figure 9. The maximum reagent diffusion, at the end of the process, for two different values of λ.

Another consequence of the chemistry is that the 'pure diffusion' phase is shorter than before (compare Figures 4 and 8); for $\lambda = 0.02$ it is negligible, while for larger values (λ=0.5) it does not differs too much with the case without the chemistry.

Concerning the behaviour of the reagent, we have to observe that its diffusion is also influenced by the parameter λ; Figure 9 shows that it increases with the micro-structural parameter. Finally, we report in Figure 10 the rupture time in function of the boundary condition c_l for several values of λ. The rupture time is obviously decreasing in c_l. A very interesting feature is the fact that we can observe a sort of threshold behaviour: beyond a certain critical value of the boundary concentration c_l, which depends on λ, the rupture time decreases very fast. In particular, we observe that in Figure 10, the curve for $\lambda = 0.1$ is different from those obtained for $\lambda = 0.01$ or in absence of microstructural effects ($\lambda = 0$). Actually, we notice that its slope decreases when the breaking time is still far from zero, and so the decay is not so fast for higher values of the reagent concentration. This could be due to the effects of microstructure that make the damage accumulation process spreadi over the specimen, increasing the rupture time. Actually, as shown by Table 5, the dependence of the blow-up time on the microstructure parameter is strongly influenced by the concentration of chemical aggression on the boundary.

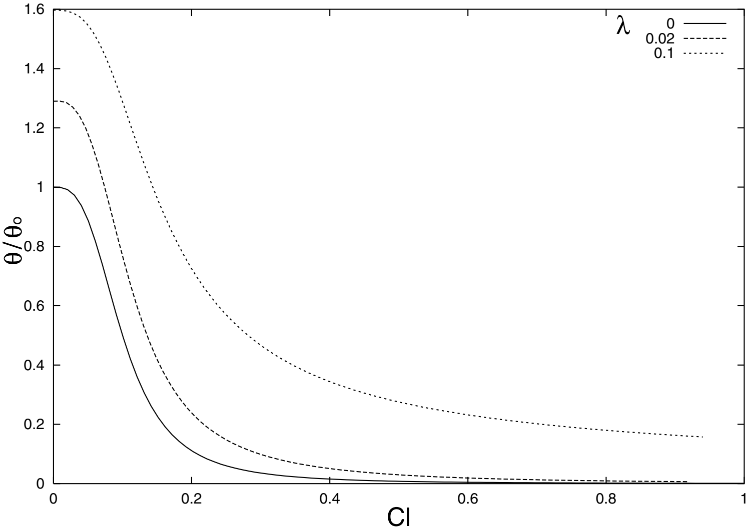

FIGURE 10. The rupture time as a function of the boundary concentration of reagent c_l, for three different values of λ (0, 0.1, 0.02).

5 Conclusions

We can summarize our results by observing that, under the chemical aggression, we have recovered all the principal features of the model without chemistry, but with a strong acceleration of the processes. The rupture set is changed by the reagent, in the sense of the concentration of the damage. However, as shown in Figure 10, the rupture time should decreases suddenly, when the boundary concentration c_l increases beyond a certain value.

Our model is clearly too simplified for including all the realistic features of the problem, and further developments should be given towards multidimensional and realistic implementations with non-trivial geometries.

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References

[1] BARENBLATT, G. I. *Private communication.*

[2] BARENBLATT, G. I., ENTONOV V. M. & RYZHIK V. M. (1990) *Theory of fluid flows through natural rocks.* Kluwer Academic.

[3] BARENBLATT, G. I. & PROSTOKISHIN, V. M. (1993) A mathematical model of damage accumulation taking into account micro-structural effects. *Euro. J. Appl. Math.* **4**, 225–240.

[4] BAZANT, Z. P. (1987) Why continuum damage is non local: justification by quasi-periodic microcrack array. *Mech. Res. Comm.* **14**, 407–419.

[5] Bertsch, M. & Bisegna, P. (1997) blow-up of solutions of a nonlinear parabolic equation. *Euro. J. Appl. Math.* **8**, 89–123.

[6] Charlwood, R. G. (1994) A review of alkali-aggregate reaction in hydro plants and dams. *Hydropower & Dams*, **1**.

[7] Crouch, R. S. & Wood, J. G. M. (1990) Damage evolution in AAR affected concretes. *Eng. Frac. Mech.* **35**, 211–218.

[8] Gottlieb, S., Shu, C. & Tadmor, E. (2001) Strong stability-preserving high-order time discretization methods. *SIAM Rev.* **43**, 89–112.

[9] Kachanov, L. M̃. (1958) On the life-time under creep conditions. *OIzvestiya (Bull.)* **8**, 26–31.

[10] Kachanov, L. M̃. (1958) Rupture time under creep conditions. In: Radok, J. R̃. M̃. (Ed.), *Problems of Continuum Mechanics*, pp. 202–218. SIAM.

[11] Kachanov, L. M. (1986) *Introduction to Continuum Damage Mechanics*. Martinus Nijhoff.

[12] Le Bellego, C., Pijaudier-Cabot, G. & Gerard, B. (2001) Coupled mechanical and chemical damage in concrete structures. In: Benallal, A. (Ed.), *Continuous Damage and Fracture*, pp. 397–407. Elsevier.

[13] Le Bellego, C., Gerard, B. & Pijaudier-Cabot, G. (2001) Mechanical analysis of concrete structures submitted to an aggressive water attack. In: De Borst, R., Mazars, J., Pijaudier-Cabot, G. and Van Mier, J. (Ed.), *Fracture Mechanics of Concrete Structures, vol 1*, pp. 239–246. Balkema.

[14] Nielsen, A. (1994) Development of alkali-silica reactions in concrete structures with time. *Cement & Concrete Res.* **24**, 83–85.

[15] Nitsch, C. PhD Thesis (in preparation).

[16] Odquivist, F. K. G. & Hult J. (1966) Some aspects of creep rupture. *Arkiv für Physik*, **19**, 379–382.

[17] Pijaudier-Cabot, G. & Bazant, Z. (1987) Nonlocal damage theory. *J. Eng. Mech. ASCE*, **113**, 1512–1533.