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Modelling and simulations of the chemo-mechanical behaviour of leached cement-based materials: Interactions between damage and leaching

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ABSTRACT

The assessment of the durability of cement-based materials, which could be employed in underground structures for nuclear waste disposal, requires accounting for deterioration factors, such as chemical attacks and damage, and for the interactions between these phenomena. The objective of the present paper consists in investigating the long-term behaviour of cementitious materials by simulating their response to chemical and mechanical solicitations. In a companion paper (Stora et al., submitted to Cem. Concr. Res. 2008), the implementation of a multi-scale homogenization model into an integration platform has allowed for evaluating the evolution of the mineral composition, diffusive and elastic properties inside a concrete material subjected to leaching. To complete this previous work, an orthotropic micromechanical damage model is presently developed and incorporated in this numerical platform to estimate the mechanical and diffusive properties of damaged cement-based materials. Simulations of the chemo-mechanical behaviour of leached cementitious materials are performed with the tool thus obtained and compared with available experiments. The numerical results are insightful about the interactions between damage and chemical deteriorations.

1. Introduction

The service life of cement-based materials, which can serve as engineering barriers for the disposal of long-term nuclear waste, is affected by different deterioration factors, such as chemical attacks and mechanical damage. The present paper is focused on the modelling and simulations of two particular sources of degradation that may interact with each other and have detrimental consequences on concrete underground facilities: (i) dissolution–precipitation reactions caused by ionic migration, governed by the material transport properties, between the interstitial solution and ground water; and (ii) damage due for instance to external mechanical loadings.

Various experimental studies evidence significant negative interactions between these deterioration factors. For example, Tognazzi [1] showed the existence of highly degraded areas around notches representing artificial cracks similar to those originated by mechanical damage. Hence, the nucleation and growth of cracks in the concrete may accelerate the transport phenomena and enhance the chemical degradation process, which in turn creates an additional porosity that affects its overall mechanical behaviour. In addition, numerous investigations dedicated to the influence of calcium leaching on the residual mechanical behaviour of cement-based materials (e.g. [2–7]) have concluded on the significant reduction of their elastic moduli and residual strength. They generally consist in performing mechanical tests such as uniaxial compression or traction tests (e.g. [2,4–7]) or 3 point flexion tests (e.g. [4]), on samples previously submitted to an accelerated leaching. Other experiments, designated as "life-time", have been performed by Le Bellégo [4] and Schneider and Chen [8,9], in which a mortar or concrete beam is subjected both to a mechanical loading and a chemical attack by an aggressive solution of ammonium nitrate. These life-time experiments show in a remarkable way the significance of the detrimental interactions between chemical deterioration and damage, since they may lead to its complete rupture after only a few months [8].

The complexity of the chemo-mechanical couplings involved in the experiments mentioned just above necessitates the use of an advanced numerical tool. The French Atomic Energy Commission (CEA) has developed, in collaboration with the French National Agency for Nuclear Waste Management (ANDRA) and Electricité de France (EDF), a numerical integration platform ALLIANCES capable of simulating problems that couple chemistry, transport and mechanics [10,11]. This platform allows for a more thorough modelling of chemo-mechanical degradations compared to existing approaches (e.g. [12–15]) by gathering within the same simulation environment a code solving chemical equilibrium and a finite volume or element software dealing with transport and mechanical problems. In a companion paper [16], a multi-scale homogenization approach has already been incorporated into this platform for predicting how the mineral composition of a

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concrete material and its linear elastic and diffusive properties are affected during a leaching process. In order to accurately simulate the chemo-mechanical behaviour of decalcified cementitious materials, it is also necessary to develop and implement into this platform a model capable of estimating the effects of damage on the material diffusive and mechanical properties.

Damage being a complex non-linear dissipative phenomenon, its influence on the mechanical and diffusive properties of cement-based materials is generally evaluated in phenomenological manners among the chemo-mechanical approaches proposed in literature (e.g. [5,7,12–15,17]). With the help of simplifying hypotheses detailed later, the present paper aims at proposing a different method by incorporating an orthotropic micromechanical damage model into the ALLIANCES platform. This micromechanical approach consists basically in proposing a simple representation of cracks at a microscopic level and in computing analytically their impact on the diffusive and mechanical properties of cementitious materials through the utilization of crack density parameters [18] and of an explicit homogenization scheme [19]. In the establishment of the model, the number of material parameters to be identified has been required be as small as possible while capturing all the first-order effects. Moreover, this study takes place in the context of nuclear waste storage where radionuclide migration and radioprotection is of paramount importance. As transfer properties controlling the movement of aggressive species are considerably more impacted in the case of tension-induced microcracking than in the case of a compression-induced one due to a much larger crack opening, we only consider in the following tension-induced damage for simplicity. Then, unilateral effects due to the opening or closure of cracks, frictional effects and plasticity are neglected in the proposed model. But future improvements are in progress to avoid these strong assumptions and extend its domains of validity and application.

In the companion paper [16], the leaching process and induced stiffness reduction of a cement paste have been simulated with ALLIANCES. The additional integration of the micromechanical damage model described in this paper inside this numerical software further allows for estimating the non-linear mechanical behaviour of leached cement-based materials as well as the impact of damage on their chemical deterioration. Diverse simulations of the chemo-mechanical behaviour of leached cementitious materials are then performed and confronted with available experimental data [4] to test the predictive capability of the proposed tool in the case of tension-induced damage.

The present paper is organized as follows. In Section 2, an orthotropic damage model based on micromechanics and on a strain-based evolution law is developed and incorporated into a FE code. In Section 3, simulations of simple decalcified structures loaded in flexion are performed and confrontation of the numerical results with available experimental data [4] is carried out. In the ensuing Section, a method is proposed to account for the retroactive effects of damage on the material diffusivity. Finally, Section 5 is devoted to the simulations of life-time tests so as to complete this study about the interactions between damage and chemical deteriorations.

2. Modelling of damage of cementitious materials

Concrete damage is a complex non-linear dissipative phenomenon, which has been the subject of extensive researches (e.g. [20]). Damage in cement-based materials is generally qualified as quasi-brittle and is caused by the nucleation, growth and coalescence of microcracks. These cracks grow preferentially in certain directions depending on the loads applied thus inducing an anisotropy of the damaged material. Many models, which are more or less phenomenological, have been proposed for treating damage in concrete, one of the most popular approaches being the Mazars model [21,22]. Its success seems mainly due to its simplicity of use in a FE code and to its capacity of accounting in a simple and relatively efficient manner for the differences of behaviour of concrete in tension and in compression. It has been extended to fatigue [23] and recently to anisotropic damage [24]. Aiming at proposing a damage model that can be incorporated into a FE code, the present work adopts a hybrid approach using homogenization techniques to determine the number and nature of damage variables and the free energy for a given damage state but also revisits the main ideas underlying the models of Mazars [21,22] and Desmorat et al. [24]. The application of micromechanics for modelling damage is a promising way to relate the damaged material behaviour to its microstructure. However, relatively few micromechanically-based models have been incorporated in FE codes (e.g. [25,26]), because they are usually more difficult to handle than phenomenological models especially in anisotropic cases.

The ensuing simplifying assumptions are adopted. The undamaged material is considered to be isotropic. The assumptions of small strains and of isothermal conditions are adopted. As already mentioned in the introduction, damage in cement-based materials being quasi-brittle, plasticity may be neglected for simplicity at least in tension, and only tension-induced damage is presently considered, so that the unilateral effects due to the opening or closure of microcracks and the frictional effects are neglected. Further developments and improvements of the model will then consist in taking into account compression-induced damage and residual strains. Note that long-term phenomena like creep may also be of importance in the context of nuclear waste disposal since the service life of storage structures is expected to be of several thousands of years.

As noticed by He and Curnier [27], a damage model within the framework of continuum damage mechanics (e.g. [28]) is generally composed of three parts. First, the damage variables are chosen to characterize as accurately as possible the defects (cracks, voids) of the concerned material. Second, the material behaviour is formulated for a given damage state. For this purpose, homogenization techniques are employed to remedy the lack of uniformity in formulating the free energy function. The evolution laws of the damage variables for a loading history are then established in Section 2.3.

2.1. Definition of state variables

The state variables are defined as the group of variables which current values characterize the physical state of a system at equilibrium. Only mechanical state variables are presently considered. The state variables are constituted of the macroscopic strain $\bar{\varepsilon}$ associated with the stress $\bar{\sigma}$ and of parameters chosen to characterize the damaged state of the material. The basic idea used by the micromechanical models (e.g. [29]) for dealing with damage consists in representing the microcracks as penny-shaped voids. By penny-shaped it is meant a spheroid, in which the length of its revolution axis is reduced to zero. Damage variables that characterize material microdefects are the crack density parameters d_i characterizing a family i of cracks having the same normal vector $\mathbf{e}_i$ associated with the driving forces Y_{di} defined in the ensuing. More precisely, these crack density parameters introduced by Budiansky and O'Connel [18] are defined as $d_i = N_i a_i^3$, where N_i is the volume density of the family i of microcracks and where a_i is the maximum axis of the degenerated spheroid representing the microcracks of type i. The damaged material is then viewed as a homogeneous matrix of cement-based material in which the microcracks are distributed. The idea of modelling these cracks as penny-shaped spheroids permits to account in an intuitive manner for the anisotropy caused by loads.

2.2. Micromechanical estimations of the damaged material behaviour

In the case of a strain formulation, the Helmhotz free energy practically corresponding to the energy stocked by elastic strains is written as:

$$\Phi = \frac{1}{2}\bar{\varepsilon} : \mathbb{C}^*(d_i) : \bar{\varepsilon}, \tag{1}$$