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Coupled carbonation-rust formation-damage modeling and simulation of steel corrosion in 3D mesoscale reinforced concrete

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ABSTRACT

This paper presents a modeling strategy to simulate the corrosion of steel reinforcement in atmospheric environment due to carbonation of concrete. Its principal objectives are to analyze the effects of the progressive formation of corrosion products at the steel/concrete interface on concrete cover cracking. The approach is based on modeling studies carried out independently on carbonation, corrosion and creep. These models are coupled and integrated into a numerical 3D simulation procedure for investigating the behavior of concrete mesostructures. A viscodamage model is used to reproduce both creep and damage behaviors of mortar, and the approach is applied to the simulation of a 3D reinforced concrete mesostructure including explicitly the coarse aggregates. The numerical results highlight the influence of aggregates and the effects of creep on crack initiation and propagation.

1. Introduction

During the service life of reinforced concrete structures, one of the main causes leading to mechanical damage in the medium and long term, is the corrosion of steel reinforcement. This process is inevitable because of the porous structure of the material which allows substances such as oxygen and carbon dioxide penetrating in the matrix concrete (see e.g. [1]). From the phenomenological point of view, the transformation of a portion of the steel section into rusts reduces its effective area and then its reinforcement properties. Furthermore, since corrosion products have a volume of 3 to 7 times greater than the initial volume of the steel lost (see e.g. [2–4]), the corresponding expansion may generate tensile stresses important enough to disrupt the concrete cover and initiate internal cracks that propagate from the steel/concrete interface to the exposed surface. The consecutive physical modifications (related both to mechanical and transport properties) then affect the durability of structure.

For structures exposed to the atmospheric environment, corrosion relates mainly to the carbonation of concrete cover. Steel in concrete is protected initially against active corrosion by a film of iron oxides on the surface of the embedded steel which prevents the dissolution of iron. Once carbon dioxide in the atmosphere penetrates in the cementitious matrix and reacts with portlandite $Ca(OH)_2$ and other hydrates as C–S–H, concrete interstitial solution is chemically modified (see e.g. [5]). When this process reaches the surface of steel and drops the concrete pH around reinforcement, the passive film disappears and active corrosion of steel occurs. The kinetics of corrosion can then change over several orders of magnitude compared to the passive state.

To take into account the corrosion in the calculation of long-term behavior of existing structures, most numerical models are developed at the macroscopic scale and then calibrated on experimental tests. This approach requires certain data about the elastic properties of the layers of corrosion products, such as the Young modulus E and Poisson ratio ν. However, these data are not yet well characterized, especially the value of the elastic modulus of rust. In the modeling, some authors consider that the corrosion products are mainly composed of water. For instance, in [6] the mechanical properties of water are adopted to represent those of the rust. The bulk modulus and Poisson ratio ν are taken to 2 GPa and 0.49, respectively. In [3] it is assumed that the corrosion products have the same properties as sound steel, and E and ν are equal to 210 GPa and 0.3, respectively. Other numerical studies calibrate the Young modulus by inverse analysis on finite element (FE) simulations such that the calculated time of appearance of scaling or amount of rust required for cracking coincides with that reported in the experimental tests. In [7,8] this value varies between 0.06 GPa and 0.15 GPa for accelerated corrosion in laboratory, and similar values ranging between 0.1 GPa and 0.5 GPa have been found in [9].

On the other hand, for natural corrosion mechanical tests on steel samples corroded in the concrete of a seaport during a time span of 40 years have been carried out in [10], revealing a modulus between 0.1 GPa and 0.6 GPa. By contrast, in a recent study of archeological artifacts over 600 years [11], the authors obtain Young modulus by micro-indentation between 70 GPa and 200 GPa. At the microscopic scale, some authors assume that the properties of the corrosion products are those of their components. For instance, [12] propose a modulus

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between 50 GPa and 200 GPa corresponding approximately to that of oxide crystal modulus. Similarly, [13] identified this parameter by oedometer tests completed by Hertz contact law on lepidocrocite and α-Fe2O3, and reported very high values between 300 GPa to 400 GPa. The experimental method also plays an important role: the last referenced study shows that the Young's modulus determined by ultrasonic measurements on lepidocrocite is two orders of magnitude smaller (0.6–5 GPa). Some data found in the literature are reported in Fig. 1.

This short review raises naturally some questions about the mechanical properties of rust. Indeed, experimental studies reporting high values of modulus were performed on samples taken from structures under natural corrosion during tens or hundreds of years [11,13]. Corrosion products are in this case well-crystallized layers, and the qualitative characterization shows that rusts contain mainly magnetite, lepidocrocite and goethite. By contrast, for accelerated corrosion tests carried out in laboratory, lower values are obtained [8–10,13]. In [9], the authors estimate that the low-crystallized products (assumed to be $FeO_x(OH)_{3-2x}$ with x equal to 0 or 1) occupy up to 45–65% of total weight of the corrosion products. During these artificial corrosion tests, it has also been observed that green rusts appear at first, then they transform into classical products such as lepidocrocite and akaganeite [14]. The existence of these unstable intermediate phases and green rusts in corrosion was cited by several studies, see e.g. [15–18]. These products contain iron oxides with valence II/III and oxidize easily to become different iron oxides with higher valence according to environmental conditions. As they progressively transform into other stable rusts, they are rarely observed in studies of archeological corrosion as noticed e.g. in [19]. However, their presence during natural corrosion in medium term seems to play a significant role in the mechanical behavior of corroded reinforced concrete because their mechanical characteristics are several orders of magnitude smaller than the ones of crystallized corrosion products.

For this reason, we propose in this study to model the development of corrosion due to carbonation of concrete in atmospheric environment based on a simplified hypothesis on the mesoscopic composition of corrosion products. We assume this latter as a two-layer composite: a first layer with low-crystallized phases containing unstable products and possibly green rust, and a second stable layer composed of well-crystallized rust, as experimentally observed in e.g. [18]. At first, steel oxidizes and transforms into unstable mobile corrosion products with low mechanical properties. These compounds then diffuse through the stable corrosion layer, re-oxidize in contact with oxygen migrating from the exterior, crystallize and become part of this well-crystallized layer. This latter comprises all the classical corrosion products: magnetite, goethite and lepidocrocite, and is assumed to be located next to the interface of virgin steel and to have a higher elastic modulus. This lamellar arrangement of the corrosion products layers allows describing in a simplified way a progressive evolution of the overall mechanical properties of rusts. This model is integrated into a coupled carbonation–corrosion–creep–damage model, which aims at simulating the response and crack initiation of reinforced concrete structure at the mesoscale. In this approach, the transport of both oxygen and carbon dioxide gases from the exposed surfaces to the steel occurs through the partially saturated connected porosity of the matrix. The kinetics of corrosion takes into account oxygen reduction and oxygen diffusion whose properties are function of water saturation degree [20]. The concrete cracking is reproduced via an isotropic damage variable [21]. To account for the creep phenomenon occurring at mid and long term, a linear viscoelastic model is introduced and coupled to the damage approach [22]. The resulting carbonation – rust formation – mechanical formulation is then implemented into the finite element code Cast3m [23] and applied to the simulation of a 3D concrete numerical sample exhibiting four phases: the matrix mortar, elastic aggregates, corrosion layer and steel rebar. The impact of the parameters introduced in the rust formation model on the time evolution of the corrosion products' thickness is then analyzed, and the time of initial concrete cracking is estimated.

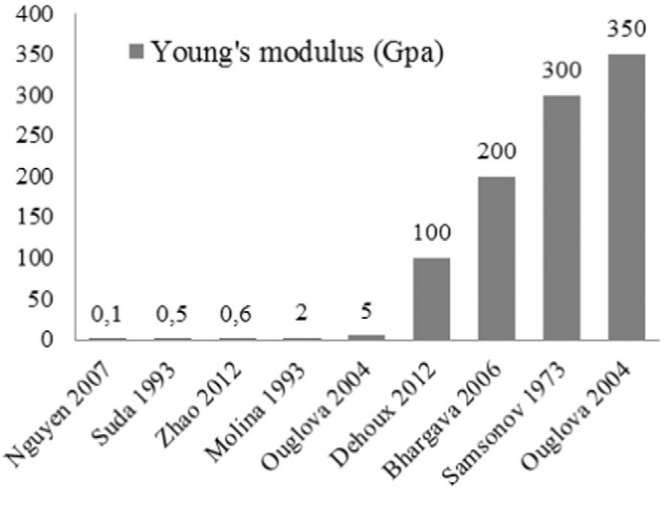

Fig. 1. Young modulus of corrosion products for different references.

2. Modeling

2.1. Coupled carbonation and drying models

We briefly recall in this section the atmospheric carbonation modeling used in our approach. The coupled drying and carbonation of concrete are described by a simplified model, initially proposed in [24] and modified and improved in [25] and [26]. This model assumes that the main phenomena involved in the carbonation are the water transport through the connected porosity, the diffusion of carbon dioxide in the gaseous phase and its dissolution followed by the reaction with portlandite and other hydrated phases to form calcite. The formulation rests on two coupled nonlinear mass balance equations for the water and the carbon dioxide in gaseous phase, respectively, expressed as [26]:

$$\frac{\partial((1-S_r)\phi P_{\bar{c}})}{\partial t} = \nabla\left[D_{CO_2}\nabla(P_{\bar{c}})\right] + W_{CO_2} \qquad (1)$$

$$\frac{\partial(\rho_l \phi S_r)}{\partial t} = \nabla\left[K(\phi)\frac{\rho_l}{\eta}k_r(S_r)\nabla(P_l)\right] + W_{H_2O}. \qquad (2)$$

These equations are governed by the pressure of liquid water P_l and the carbon dioxide pressure $P_{\bar{c}}$, respectively. Note that in Eq. (2) it is assumed that the transport process for moisture results only from water pressure gradients, meaning that the diffusion of vapor in gas phase is disregarded. Furthermore, the pressure of the gas phase is neglected with respect to the one of the liquid, such that $P_c \approx -P_l$, with P_c the capillary pressure. Another remark is that the CO_2 is assumed to behave as an ideal gas, which implies the relation $\rho_{\bar{c}} = M_{\bar{c}} P_{\bar{c}}/(RT)$, with $\rho_{\bar{c}}$ and $M_{\bar{c}}$ the density (kg m^{-3}) and molar mass (kg mol^{-1}) of CO_2, respectively, R is the perfect gas constant (8.31 J mol^{-1} K^{-1}) and T is the temperature assumed constant ($T = 293$ K). In Eqs. (1)–(2), ϕ is the porosity of concrete, S_r is the saturation degree relative to the total porosity and D_{CO_2} is the effective diffusion coefficient of CO_2 (m^2 s^{-1}). This last parameter is chosen to evolve as a function of the relative humidity h_r via the empirical function proposed in [27,28] as $D_{CO_2}(h_r) = A_{CO_2}(1-h_r)^{n_{CO_2}}$, where A_{CO_2} and n_{CO_2} are adjusting parameters. W_{CO_2} stands for the source term related to the dissolution of CO_2 in the liquid phase and precipitation of calcite, ρ_l is the density of water, $K(\phi)$ is the intrinsic permeability coefficient depending on the porosity, η is the dynamic viscosity of the water (0.001003 Pa.s), $k_r(S_r)$ is the relative permeability to water, and W_{H_2O} is the water source term. The expression of the different