NUMERICAL MODELLING OF AUTOGENOUS HEALING AND RECOVERY OF MECHANICAL PROPERTIES IN ULTRA-HIGH PERFORMANCE CONCRETE

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ABSTRACT

Cracks, caused by shrinkage or external loading, reduce the durability of concrete structures as aggressive substances can easily enter in the capillary network of the cementitious matrix. Natural 'autogenous' healing ability of concrete by further hydration or precipitation has been studied experimentally for many years. Autogenous healing of concrete by further hydration of residual unhydrated cement particles is triggered by the ingress of water and/or moisture into the crack and leads to a partial recovery of mechanical properties (Young's modulus, tensile strength,...). However, theoretical studies and computer simulations still need to be developed in order to explain macroscopic behaviour of healed specimens and conditions of occurrence of the self-healing phenomenon.

In this study, a hydro-chemo-mechanical model was developed to simulate autogenous healing by further hydration. Firstly, a simulation of a three-point-bending test was performed to represent the initial damaged state before the self-healing process. The volume fraction of the residual cement clinkers at this moment has been calculated with a hydration model. Then, the self-healing phenomenon of concrete beams immersed into water was modelled based on micro-mechanical observations. The diffusion process has been simulated using the Fick's law in order to describe the ingress of water into concrete. The hydration model, based on the Arrhenius law, is then used to simulate the chemical reactions between residual clinkers and water. The mechanical properties of the new formed hydrates are therefore evaluated in order to describe the partial recovery of mechanical properties of healed concrete.

1. INTRODUCTION

Cracks in concrete can heal naturally under favorable conditions. This phenomenon called 'autogenous' healing is the consequence of two main reactions depending on the concrete nature: further hydration for concrete with an important amount of unhydrated cement particles and formation of insoluble calcium carbonate when calcium contained in the cementitious matrix can react with carbon dioxide dissolved in the water filling the crack. Autogenous healing by further hydration has been studied by several researchers. Granger et al. [1] used ultra high performance

cementitious material – UHPC– with a water-to-cement (W/C) ratio close to 0.2 to study the self-healing of cracks with different widths. Mechanical properties of healed and uncracked specimens were compared at different stages (1 week, 3 weeks, 10 weeks, 20 weeks and 40 weeks). However, only few models were developed to describe self-healing of concrete and none of them described the restoration of the mechanical properties.

In this study, a hydro-chemo-mechanical model was developed to simulate autogenous healing by further hydration. The self-healing of a concrete beam was calculated after cracking in a three-point-bending test. The recovery of the cracked concrete beam was obtained by decreasing the local damage value due the fill in of empty space by new hydrates.

2. PROBLEM FORMULATION

First, three-point-bending tests were simulated on a concrete beam to represent the first experimental step corresponding to the creation of the crack, considering an anisotropic description of the damage (eq 1) [2]. Damage is defined through the relationship between the overall stress σ, the total strain $\varepsilon^{\acute{e}}$, the plastic strain ε^{p} and the local initial stiffness C^0 at each point y:

$$\sigma(y) = (1-d)C^0(y) : (\varepsilon(y) - \varepsilon^P(y)) \tag{1}$$

d represents the scalar value of the isotropic damage:

$$d = 1 - \frac{\varepsilon_{d0}}{\varepsilon_{eq}} \exp\left[B_t\left(\varepsilon_{d0} - \varepsilon_{eq}\right)\right] \tag{2}$$

where B_t represents a damage parameter to control the slope of the strain softening constitutive relation in function of the width h of the element and ε_{d0} the strain threshold. ε^p is computed using a loading function by the normality rule.

To model the autogenous self-healing, external humidity conditions are considered by the arrival of water on the boundary of the beam. The ingress of water, with a speed U, through the damaged material was simulated by using the Fick's law:

$$\frac{\partial U}{\partial T} = D(d)\frac{\partial^2 U}{\partial X^2} - kU \tag{3}$$

where D(d) represents the diffusivity coefficient depending on damage [3].

The local quantity of water inside the beam was then used to activate the hydration process which determined the volume of each component in the microstructure [4]:

$$\tau_i \frac{d\xi_i}{dt} = \tilde{A}(\xi_i) \text{ and } \quad V_k^P(t) = \sum_l^n \left(V_i^0 \frac{n_k^P M_k}{n_l^R M_l} \frac{\rho_C}{\rho_k} \right) \xi_l(t) \qquad k = 1, m \tag{3}$$

where V_i^0 represents the residual clinkers in concrete, V_k^p the new formed hydrates, M the molar mass, ρ the mass density, n the mole number and ξ_i the hydration coefficient of each clinker. The index k represents the products (clinkers), l the reactants and c the cement. $\tilde{A}$ and τ are the normalized affinity and the characteristic time, respectively, used in the Arrhenius law.

The amount of the hydration products created in the damage area fill in the empty space and decreases the local damage value.

3. RESULTS

The constitutive damage parameters used to perform the three-point-bending simulations on a notched beam were adjusted in order to fit the experimental loading curves during the stage of the creation of the crack. The selected Young's modulus is 45 GPa, tensile strength is 5 MPa and Poisson's ratio 0.2. The final crack width was equal to 10 μm. Using the damage state at the end of the first stage representing the crack creation, the healing model was applied to see the influence of the creation of new hydrates on the mechanical behaviour of concrete (fig 1). Because the water diffusion started at the bottom of the beam in the model, the new hydrates were created from the bottom to the top of the beam, and the damage diminution as well.
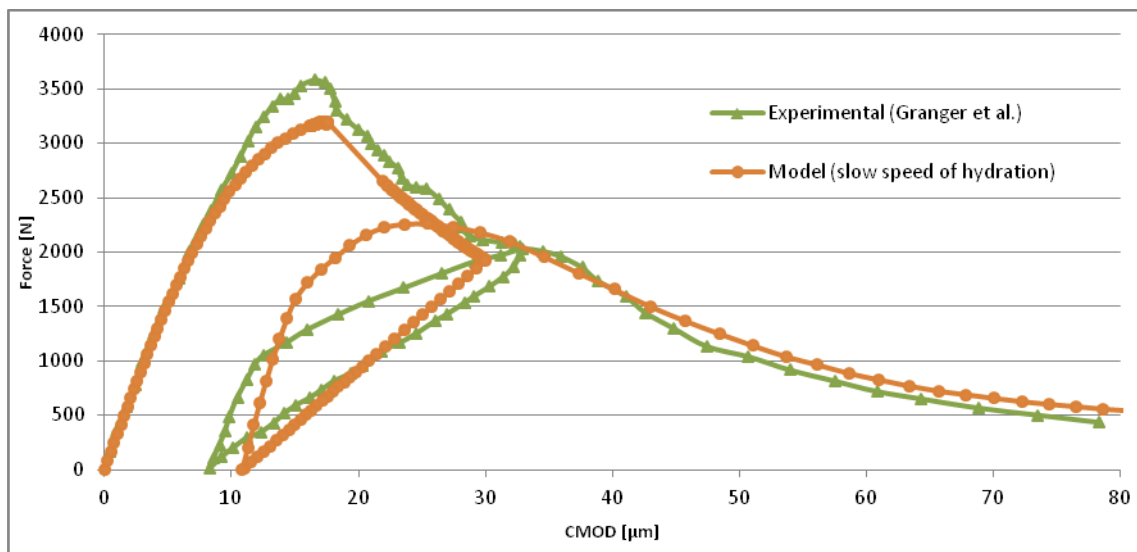

Figure 1: Numerical loading curves before and after healing in comparison with an experimental test (Granger et al., 2007).

The algorithm was applied to different times of healing, considering several speed of hydration and with the possibility to study various mechanical behaviour of the healed zone (fig 2). The simulation of the three-point-bending test after healing revealed that the mechanical behaviour of the healed beam is very sensitive to the kinetic of formation of the new hydrates. For a speed of hydration equal to that observed in concrete at early ages, the healing is almost stopped because the new hydrates are formed at the bottom of the beam and water ingress in the damaged zone is very slow because the diffusivity coefficient is small in undamaged areas. When the kinetic of formation of new hydrates is reduced, the healed zone can be larger over. The difference in the reloading (two slopes in experiments) could be due to different elastic properties and/or kinetic of hydration in the healed area. The elastic response and the maximum bearing load of the beam are affected.
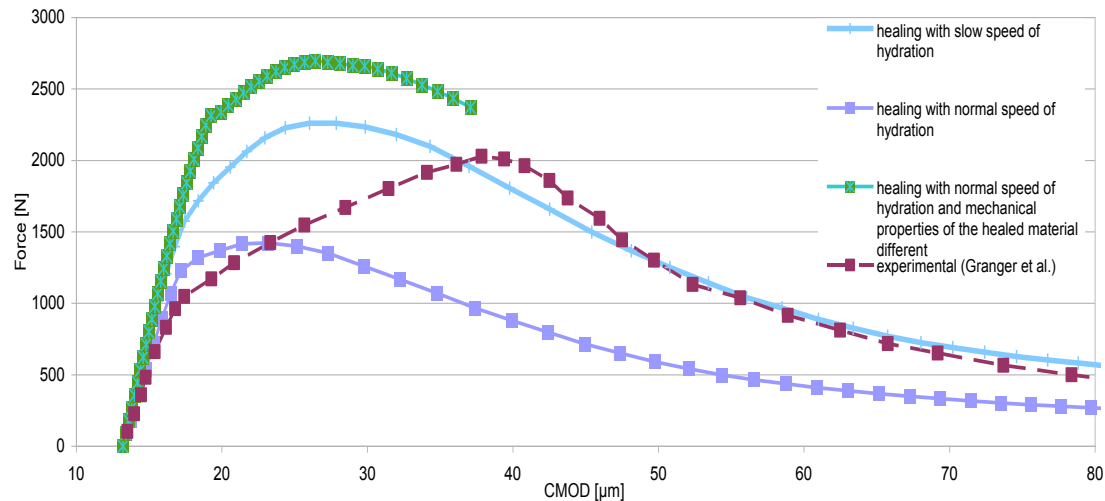
Figure 2: Numerical loading curves after healing with different speed of hydration and with different properties for the new hydrate.

4. CONCLUSIONS

Modelling the autogenous healing in concrete is still a great challenge. A numerical model could help to describe experimental observations and could also help to predict the evolution of mechanical properties of concrete structures during their service life. The speed of formation of the new hydrates in the cracked and damaged concrete seems to play an important role on the speed on healing. However, further investigations are needed to understand the recovery of mechanical properties in concrete structures as well as the occurrence of the self-healing phenomenon. Tests will be made on the influence of the elastic properties of materials in the healed area to obtain the two slopes in the reloading.

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