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MODELLING OF CREEP EFFECT ON A HEALED CRACK IN CEMENTITIOUS MATERIALS

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Abstract: Self-healing of cracks by continuous hydration of unhydrated cement particles provide an improvement of mechanical properties for cementitious materials. Recent studies indicate that concrete specimens subjected to a sustained mechanical load lead to a variability of the mechanical properties recovery during self-healing. In fact, the presence of sustained mechanical load inset the creep deformations of concrete. In this paper, a numerical model based on the coupling of the microstructural hydration code CemPP and the finite element code Cast3M was performed to describe the mechanism of creep for healed structures. Numerical simulations have been carried out to determine the mechanical regains of cement paste cracked at 48 hours and then subjected to ongoing hydration process. After this first step, the viscoelastic creep behavior was investigated by applying a tensile creep load equal to 40% of tensile strength for each healed microstructure.

1 INTRODUCTION

Cracks can originate from several phenomena such as shrinkage or creep all along the service life of a structure. Because of cracks, harmful substances can easily ingress into the concrete matrix, promoting damage in mechanical properties and thus affecting the service life. Self-healing of concrete appears to be a promising mechanism by allowing the recovery of materials' properties. The intrinsic ability of concrete to heal is described by the continuous hydration of unhydrated cementitious particles and/or the precipitation of calcium carbonate [1]. It is characterized by the reaction of unhydrated particles of clinker with water to form secondary hydration products like portlandite (CH) and C-S-H which can lead to strength and stiffness regains[2,3]. From different research works, it was found that autogenous healing potential depend on the crack width [4], the cracking age [5], the type of cementitious material and the presence of sustained mechanical load which inset the creep mechanism of concrete [6]. It should be noted that the autogenous healing mechanism is limited to small cracks and it requires the presence of water [7]. Moreover, numerical models have been carried out to describe autogenous healing of concrete by continuous hydration. They were proposed to estimate the mechanical regains and to determine the evolution of the filling fraction of cracks after duration of healing [5,8]. However, these models do not provide information about the loading and the origin of crack propagation.

On the other hand, creep deformations mainly occur in the cement gel of hardened cement paste like calcium silicate hydrates (C-S-H). The creep phenomenon of C-S-H is considered as the dominant source of creep in concrete [9]. When concrete is subjected to static load, the resulting deformation including creep deformations is much greater than elastic deformation. Therefore, it would be interesting to investigate the creep deformation of structures taking into account the self-healing process.

In this paper, a numerical investigation of the viscoelastic behavior of healed cement paste is presented. Numerical models were carried out in two sequentially phases, self-healing by continuous hydration and tensile load creep. To characterize the self-healing of cementitious materials by continuous hydration, the developed version of CEMHY3D called CemPP, which has a resolution of 1µm, is adopted [5]. Then, the healed microstructure is used as input to the finite element code Cast3M. Then, numerical tensile tests were performed to obtain the viscoelastic behavior of non-aging healed structure subjected to a static load. The model adopted in this first work does not take into account the evolution of intrinsic properties during loading.

2 CREEP / SELF – HEALING SIMULATION

2.1 Methodology and microstructure generation

The simulation of the healing process by ongoing hydration was performed in 3D by using the hydration code CemPP which is based on CEMHYD3D V3 [10]. A 40x40x40 µm^3 microstructure of cement paste was discretized into voxels with a size of 1 µm. At age of 48 h, as an experimental age of cracking, a 5 µm plane micro-crack was artificially introduced by replacing part of the microstructure by water-filled porosity and then the hydration process was restarted in order to simulate the ongoing hydration of particles around the crack.

Hydration process was modeled by dissolution, diffusion, and precipitation cycles based on reactions defined in CEMHY3D. Table 1 summarizes the input parameters for CemPP. Figure 1 shows the generated microstructures during the healing process for different hydration times. Precipitation of hydration products occurs in the crack as expected. Then, healed volumes have been saved at different healing times corresponding to the experimental healing times, and they were analyzed to determine the nature of healing products and their distribution inside the crack.

At each time of the healing process, a cross section S_i was extracted to perform micro-mechanical tests with the finite element code Cast3M [11] in order to obtain the mechanical behavior of a healed specimen knowing the intrinsic properties of the phases.

Table 1: Input parameter of the hydration model CemPP used for the simulation of the self-healing process.

Blain fineness	390 m^2/kg
Gypsum dihydrate	4.2 %vol.
Activation energy	40 kJ/mol
W/C	0.4
Curing conditions	Saturated
Initial temperature	20 °C

To do so, a first test has been performed by applying a tensile load to calculate the maximum tensile strength of the healed microstructure with consideration the damage model detailed in the next section. Then another test consisting on applying a constant tensile load on the healed microstructure to calculate the effective viscoelastic response assuming the material behaves without any damage creation was done.

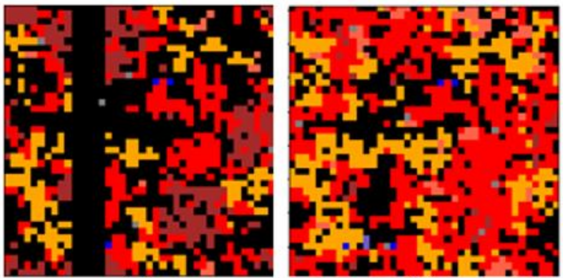
(a) (b)

Figure 1: 2D sections extracted from a virtual 3D microstructure of CemPP at a cracking age 48h (a) and at healing time 336h (b).

2.2 Mechanical properties of the individual phases: Damage model

In this section, the viscoelastic behavior calculation of healed cement pastes under a constant load is detailed. Finite element simulations have been carried out on a cross section microstructure chosen at a specific location along the direction Z (alongside the crack height) of hydrated volume generated by CemPP.

In our work, the damage model used is the isotropic model developed by [12]. It is restricted to only pure tensile loading where the load was applied as incremental horizontal displacements on one of the sides (Γ_1) of section S while the opposite one (Γ_2) is fixed. Boundary conditions are shown in Figure 2 and the scalar damage variable evolution reads:

$$D = 1 - \frac{\kappa_0}{\tilde{\varepsilon}} e^{-B(\tilde{\varepsilon}-\kappa_0)} \qquad (1)$$

Where $\kappa_0 = \frac{f_t}{E}$ is the damage threshold, E is the elastic modulus, $B = \frac{hf_t}{G_f}$ is a damage parameter to control the slope of the strain softening curve, f_t is the tensile strength, G_f is the fracture energy and h corresponds to the size of the finite element [13].

Thus, the tensile strength of the healed microstructure was determined and the global stiffness has been calculated. Therefore the model applied at the microscale described the healing efficiency at different times of healing.

It should be noted that a reference sample without crack was compared to the healed samples. It means when the material is successfully healed the tensile strength in the healed configuration tends to be similar to the tensile resistance of the reference sample.

2.3 Mechanical properties of the individual phases: creep model

Creep is modeled by a series of four chains of Kelvin-Voigt (Figure 3). The characteristic diffusion times τ_i are respectively: $\tau_1 = 0{,}1j$, $\tau_2 = 1j, \tau_3 = 10j$ and $\tau_4 = 100j$ [14]. The numerical simulations are conducted under plane stress condition. The modeled basic creep has been exploited without taking into account the damage effect.

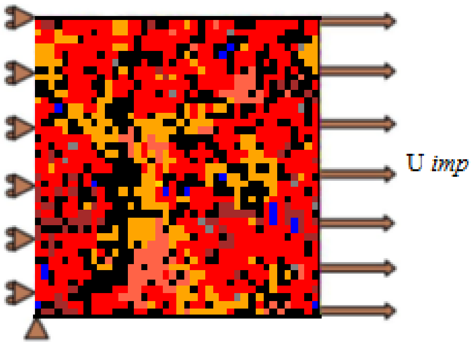

Figure 2: Boundary conditions applied on a healed 2D section of cement paste.

A unidirectional constant loading equal to 40% of the maximum tensile strength of healed cement paste was applied (Figure 4). The numerical resolution of the viscoelastic problem was performed to determine the effective viscoelastic response of healed materials for different times of the healing process. The effective creep tensor based on the relation between the average deformation and the average stress is given by [14]:

$$\varepsilon^f = J(t).\sigma(t) \qquad (2)$$

The micromechanical properties of cementitious phases are obtained by an inverse analysis detailed in [13].

An overview of the CemPP–Cast3M coupling is represented in Figure 5.

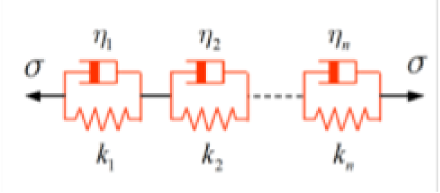

Figure 3 : Creep model by Kelvin-Voigt chains.

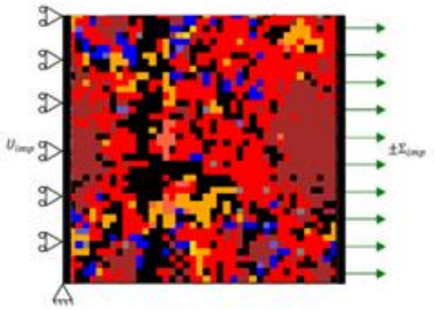

Figure 4: Boundary conditions applied to a healed cement paste section.

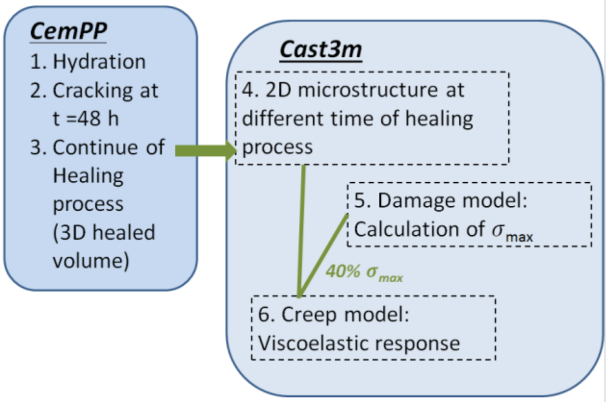

Figure 5: Overview of the numerical simulation coupling CemPP & Cast3M.

3 NUMERICAL RESULTS AND DISCUSSION

3.1 Strength of healed microstructures

Figure 6 shows the numerical strength recovery that occurred due to healing for specimens subjected to healing process durations as a percentage of the strength of the corresponding uncracked specimens exposed to the same process without being cracked at 48 h. In this figure, a strength recovery capacity due to healing by ongoing hydration appears slightly around 120h and increase progressively to reach 55% of the strength of the reference sample after a 166-days immersion.

This can be attributed to the continuous hydration of anhydrous cement particles present on the crack which leads to a precipitation of healing products that contribute mechanically to bridge the two faces of crack. It is also observe that self-healing capacity grows with increasing the duration of curing in water for cracked specimen.

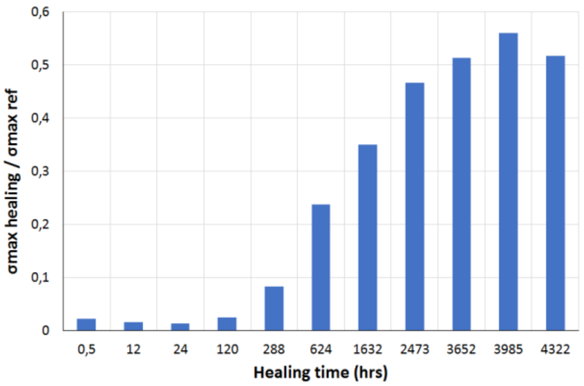

Figure 6: Numerical influence of healing durations on strength recovery for specimen with a 5µm wide crack (cracked at 48h).

3.2 Evolution of creep properties with healing

The numerical creep tests are presented in Figure 7. In this study we have chosen to test the creep deformation of the healed microstructure and the reference sample with a similar load level equal to 40% of the maximal strength of healed microstructure. The numerical creep displacement obtained for the healed microstructure is higher than creep displacement for reference sample which is expected. In case of the reference sample, the applied tensile load was found smaller than 40% of its own maximal strength with range between 8 to 51%.

In fact, the solidification process of cement by hydration reactions leads to increase the volume fraction of C-S-H gel with age. Figure 8 shows that creep deformations for 4033h of healing is greater than deformations obtained for 3700h and 1680h of healing. The increasing of creep at age is attributed to the gradual formation of C-S-H due to hydration process which indicates that C-S-H phase is responsible for microscopic creep deformation. The applied stress is redistributed to the newly formed cement gel which causes the relaxation of the transversal micro-stress [15].

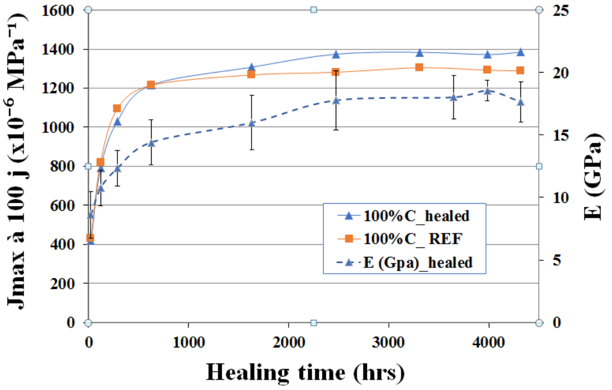

Figure 7: Comparison of specific creep for healed cement paste (plain blue curve) and reference sample (plain orange curve) at different times of healing (per hours), and elastic modulus evolution of the healed microstructure (Dotted blue line).

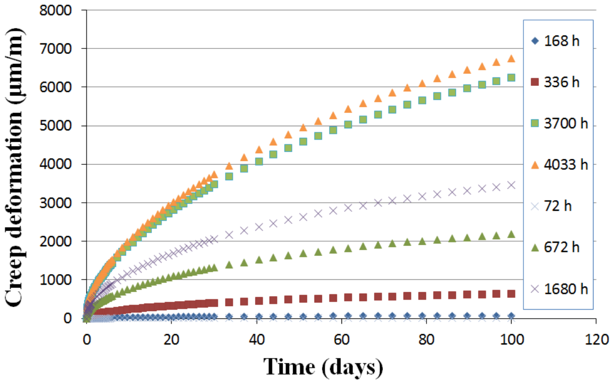

Figure 8: Basic creep displacements for healed cement paste at different time of healing

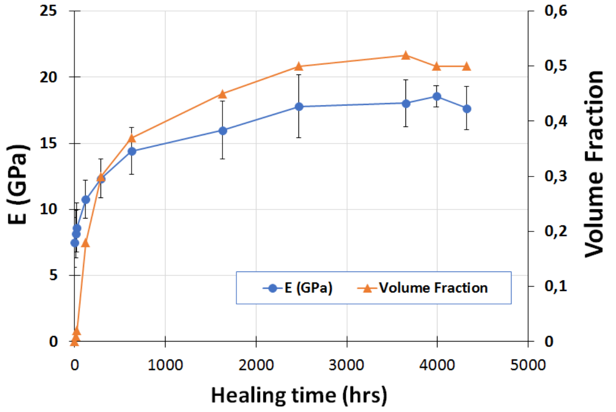

Figure 9: Numerical stiffness regains due to the crack healing and filling fraction of the crack.

Therefore, the numerical E-modulus for cracks created at 48h seems to increase at early age and then stabilizes at a later with an advanced age (Figure 7). These results correlated well to the properties evolution of cement paste. In fact, with continuous hydration the healing products form bridges that are responsible for stiffness regains of cement paste structure [5]. As shown in Figure 9, the elastic modulus tends to linearly increase with the volume fraction of healing products due to bridges of hydrates crosses the crack. The very fast stiffness regains appear at an early age can be explained by the hydration of particles smaller than 1µm [5].

4 CONCLUSIONS AND PERSPECTIVES

In this study, the microscopic creep of healed cement pastes has been studied. The results show a very good mechanical regains (stiffness and strength) can be obtained for small cracks with a width of 5 µm when they are created at 48h. Tensile creep tests were performed after different healing periods by adapting the load at each time. According to the results of the simulation, the amount of C-S-H formed is correlated to the creep deformations.

While this promising model provides some information about the self-healing and creep coupling, additional applications of the model could be developed to better understand the creep mechanism for healed structures. Several supplementary studies could help representing the phenomenon by taking into account new parameters in which the description of healing systems when sustained load is applied would be more representative.

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