Numerical investigation of the mechanical behaviour of a structural element containing a self-healing agent

T Zhelyazov¹⁻³ and R Ivanov²

¹ Department of Mechanics, Faculty of Transport, Technical University of Sofia, 8 Kl. Ohridski Blvd., Sofia 1000, Bulgaria
² Section “Seismic Engineering”, Department “Seismology and Seismic Engineering”, National Institute of Geophysics, Geodesy and Geography – Bulgarian Academy of Sciences, Acad. G. Bonchev St., bl. 3, Sofia 1113, Bulgaria
³ E-mail: todor.zhelyazov@tu-sofia.bg

Abstract. This paper presents a virtual experiment on the behaviour of a self-healing material from the family of cement-based composites, that contains a healing agent. A numerical model of a specimen made of a cement-based material, and containing a healing agent is subjected to the loading configuration of the four-point bending test, whereby the forces are applied in a quasi-static way. The response of the healed specimen is compared to the response of a specimen that doesn’t contain a healing agent. For the specimen that contains a healing agent, homogenization techniques are used to determine the characteristics of the equivalent material (cement-based composite / healing agent) in zones where damage and macro-cracking have occurred, i.e., zones in which the healing agent has been activated. The main result of this contribution is the formulation and validation of a numerical simulation approach suitable for modelling the mechanical behaviour of self-healing cement-based composites.

1. Introduction

Increasing demands in exploitation along with the desire to extend the service life of structures, machines, and vehicles boost the research in many fields of industry and science. Material science provides new materials and advanced techniques for refurbishment, such as self-healing. For example, ceramic–matrix composites gain positions as structural components of hypersonic and rocket engines [1], cement-based composites for strengthening or repair of structures [2]. Significant research has also been done on the use of nanomaterials for enhancement of the performance of composites [3]. Self-healing is a technique for refurbishment applicable to a wide range of materials, such as metals [4], asphalt [5], etc.

Concrete has been known to possess self-healing properties ever since it became widely used as a construction material more than a hundred years ago. The concept of self-healing is a very appealing one, since it offers a way of overcoming the inherent flaw of concrete structure to develop cracks due to various reasons followed by gradual structural deterioration. Following the first formal report on self-healing concrete, [6] the research on the subject has been very active, [7] and references therein. The two mechanisms by which self-healing occurs – autogenous and autonomous have been identified and research has been conducted in both directions encompassing all physical phenomena and technological challenges involved, e.g. hydration and crystallization and the water supply needed for
it, healing by epoxy resins, the delivery of healing agent by capsules, the role of moisture air and heat in the healing process, the reaction of the healing agent with the cementitious matrix or with a hardener, vascular systems for healing agent delivery etc., and their efficiency and feasibility, [7, 8]. Research on numerical simulation methods to complement the experimental investigations has followed suit and has been equally diverse, [9]. Most notably, a coupled hydration – elastic damage model has been developed and used to simulate a three-point bending test of a concrete specimen, [10], a model incorporating all relevant material behaviour such as mechanical damage, creep, shrinkage, thermal effects, self-healing and the interactions among the is presented in [11]. The fracture behaviour of encapsulation-based self-healing concrete is studied in [12], whereby the influence of parameters such as the volume fraction of capsules, and their shell thickness is incorporated. In [13], the Solidification-Microprestress-Microplane model for concrete has been extended to apply to self-healing and used to simulate the recovery of mechanical properties in cement-based composites.

The aim of this contribution is to demonstrate how a Damage Mechanics based computation incorporated into finite element code, can be extended and used to assess the effect of self-healing on the behaviour of a structural member made of cement-based composite, subjected to mechanical loading.

2. Finite element modelling

A four-point bending test is simulated. The model is 0.40 m long, 0.10 m deep and 0.10 m wide, the span is 0.30 m, and the two loading lines are at 0.10 m from the model mid-point, figure 1.

The finite element mesh and the support conditions are shown in figure 2.

Figure 1. Geometry of the test specimen (all dimensions are in millimetres).

Figure 2. Finite element model of four-point bending test.
The loading is applied stepwise as prescribed displacements to the relevant nodes on the top surface of the model, thus simulating a displacement-controlled test. All nodes of the two supports are restrained in the global \(Y\) direction. In order to prevent rigid body motion, one node of the left-hand support is restrained in the global \(X\) and \(Z\) directions, while one node of the right-hand support is restrained in the global \(Z\) direction.

The cement-based composite has an initial modulus of elasticity \(E\) (of the undamaged material) of 29,000 MPa and a Poisson’s ratio \(\nu\) of 0.22. The mechanical characteristics of the healing agent are as follows: \(E_h = 7,050\) MPa and \(\nu_h = 0.39\).

The cement-based composite is assumed to have fragile, strain-softening behaviour which is modelled by coupling linear isotropic elasticity with damage [14]:

\[
\sigma_{ij} = \frac{\nu}{(1+\nu)(1-2\nu)}E(1-D)\varepsilon_{kk}\delta_{ij} + \frac{1}{(1+\nu)}E(1-D)\varepsilon_{ij}
\]

In equation (1), \(\varepsilon_{kk}\) is the trace of the strain tensor \(\varepsilon_{ij}\), and \(\delta_{ij}\) are the components of the unit tensor. The scalar damage variable is split into a tensile, and a compressive component [15]:

\[
D_t = 1 - \frac{\varepsilon_{inf}(1-A_t)}{\varepsilon_{eqv}} - \frac{A_t}{\exp[B_t(\varepsilon_{eqv}-\varepsilon_{inf})]}
\]

\[
D_c = 1 - \frac{\varepsilon_{inf}(1-A_c)}{\varepsilon_{eqv}} - \frac{A_c}{\exp[B_c(\varepsilon_{eqv}-\varepsilon_{inf})]}
\]

The material constants \(A_t, B_t, A_c, B_c\) and \(\varepsilon_{inf}\) should be identified via curve fitting. The equivalent strain \(\varepsilon_{eqv}\) is defined as follows:

\[
\varepsilon_{eqv} = \sqrt{\langle \varepsilon_1 \rangle^2 + \langle \varepsilon_2 \rangle^2 + \langle \varepsilon_3 \rangle^2}
\]

In equation (4) \(\varepsilon_i, (i = 1.3)\) are the principal strains, and the McAuley brackets applied to a given quantity \(q\) are typically defined as follows:

\[
\langle q \rangle = \frac{1}{2} (q + |q|)
\]

Damage accumulates provided the condition

\[
\varepsilon_{eqv} \geq \varepsilon_{inf}
\]

is met.

A subroutine is developed to implement the nonlinear constitutive relation defined by equations (1) – (4) into the general-purpose finite element code ANSYS Mechanical APDL (®, TM). The strain-softening response of the cement-based composite material is obtained by incremental finite element analysis. For each increment of the analysis, the stress and strain distributions are determined. The tension and compression components of the damage variable are calculated and for the finite elements where damage accumulation is detected (i.e., where the criterion provided by equation (6) is met), the material constants are modified, according to equation (1). Furthermore, finite elements in which the critical value of the damage variable is reached are deactivated and do not contribute to the overall rigidity of the structural member in the subsequent increments.

It is assumed that a healable crack propagates in zones where the critical value of the damage variable is reached \((D = D_{max})\). As to the relation between the loading, cracking and healing, two scenarios are considered: a) the loading rate is very slow, so a newly-formed crack is filled with healing agent which has cured completely before the next loading step, and b) the loading rate is very fast, so healing cannot take place during the loading time. Instead, healing of all cracks occurs simultaneously, and the structure is again subjected to loading only after healing has completed.

For a specified finite element, the volume of cracks is predicted by subtracting from the volume of the deformed finite element \(V_{d,FE}\) (prior to deactivation) the volume of the same finite element \(V_{l,FE}\) in the initially generated finite element mesh,
\[ V_{\text{crack}} = V_{d,FE} - V_{lFE} \]  \hspace{1cm} (7)

Finite elements containing cracks filled with healing agent are homogenized (see, for example [16]):

\[
\frac{\mu_{\text{eff}} - \mu_1}{\mu_{\text{eff}} + \mu_1} = f \frac{\mu_2 - \mu_1}{\mu_2 + \mu_1} \]  \hspace{1cm} (8)

\[
\frac{\left( \lambda_{\text{eff}} - \mu_{\text{eff}} \right) - (\lambda_1 + \mu_1)}{\lambda_{\text{eff}} + \mu_{\text{eff}} + \mu_1} = f \frac{(\lambda_2 + \mu_2) - (\lambda_1 + \mu_1)}{\lambda_2 + \mu_2 + \mu_1} \]  \hspace{1cm} (9)

In equations (8) and (9) \( \mu_1, \lambda_1 \) and \( \mu_2, \lambda_2 \) are the Lamé coefficients for the cement-based composite and for the healing agent, respectively; \( f \) stands for the volume fraction of the healing agent,

\[ f = \frac{V_{\text{crack}}}{V_{lFE}} \]  \hspace{1cm} (10)

For the considered case, for practical purposes, after the micro-crack initiation and the activation of the healing agent, the homogenization may be avoided by simply restoring the initial mechanical characteristics of the cement-based composite. In the subsequent loading, the restored mechanical properties will be maintained until the tensile strength of the healing agent is reached. This argument will hold as long as the volume of the crack is small compared to the volume of the finite element, i.e., the mesh is relatively coarse.

3. Results and discussion

A comparison between the response of a test specimen without a healing agent and a test specimen subjected to the action of a healing agent is shown in figure 3. Both specimens have the same geometry, identical mechanical properties, and are subjected to a displacement-controlled quasi-static loading.

![Figure 3](image1.png)

**Figure 3.** Evolution of the mid-span deflection of a specimen without healing agent and a specimen with healing agent. Absolute values of the mid-span deflection are plotted. According to the convention for the coordinate system used (see figure 1), the mid-span deflection should be negative.

![Figure 4](image2.png)

**Figure 4.** The predicted effect of the healing agent: comparison between the mechanical responses of a specimen containing a healing agent and a specimen without a healing agent. Absolute values of the mid-span deflection are plotted.

It can be seen that with the damage accumulation and cracking, the specimen which is not subjected to the action of a healing agent loses rigidity, which results in a more rapid increase of the mid-span deflection. The same trend is confirmed by figure 4 from a different perspective; with the loading and the healing action being concurrent, the specimen preserves its load-bearing capacity much better than its non-healing counterpart.
Both figure 3 and figure 4 illustrate the continuous action of the healing agent. The healing agent starts to act as soon as the cracks’ width reaches a specific, predefined value (equivalent to a specified value of the damage variable in the model). The healing agent fills the macro-crack as soon as it forms ($D = D_{\text{max}}$). It should be noted that this scenario can be considered realistic only for a loading rate smaller than the curing rate of the healing agent.

Figure 5 illustrates another loading scheme. The test specimen is loaded until a specified amount of damage is reached. The specimen is then unloaded and healed. Afterwards, the specimen is loaded again. The mechanical response shown in figure 5 is obtained for a different set of model constants ($A$, $B$, $A_e$, $B_c$).

![Figure 5. Mechanical response of specimens, subjected to partial healing after a preloading phase. Absolute values of the mid-span deflection are plotted.](image)

The healing process is illustrated in figure 6 and figure 7. During loading, mechanical damage is initiated and accumulated in the specimen, which results in a degradation in the initial mechanical properties of the material. This can be seen in figure 6, where all finite elements affected by damage, i.e., all finite elements in which Young’s modulus has become less than the initial one, because of damage accumulation are plotted in light blue. Due to the action of the healing agent, the initial mechanical properties are partially restored. Figure 7 shows the damaged specimen from figure 6, after having been subjected to partial healing. Again, finite elements of degraded material properties are plotted in light blue, whereas finite elements in which the initial material properties are maintained (or restored due to the action of the healing agent) – in blue.

![Figure 6. Damaged specimen. All finite elements affected by damage are displayed in light blue.](image)

![Figure 7. Partially healed specimen: the initial mechanical properties of some of the damaged finite elements are restored.](image)

It should be noted that the model chosen for the cement-based composite is not designed to account for the damage-induced anisotropy; a scalar damage variable is used in the constitutive relation.

It has been pointed out above that after the micro-crack initiation, the healing agent is activated and fills immediately the newly-formed crack when the limit value of the damage variable is reached. At this point, the medium within the finite element is relieved from stress due to the formation of a macro crack, which is healed once the agent cures, so a portion or all of the initial rigidity of the medium should be restored. How much should be restored is a question that can only be clarified by experimental evidence.
Typically, it is assumed that damage localization takes place. However, if damage localization is considered as a process, any formation of a micro-crack is equivalent to formation of a damaged zone within the finite element. The healing agent acts only in the finite elements in which the value of the damage variable is larger than a specific value, i.e., it is tacitly assumed that the healing agent cannot circulate in cracks of width less than a specified value. Thus, the restored rigidity within the finite element should be inferior to the initial characteristics of the material at this location.

As pointed out, the input for the strain-softening model is provided by the strain distribution obtained for each increment of the nonlinear finite element analysis. In the context of this study, the stress distribution is relevant only for the investigation of possible failure in the joint formed by the healing agent after the partial healing. The first principal stress determined in the healed finite element is compared with the tensile strength of the healing agent. The stress distributions for two consecutive increments of the numerical simulation are plotted in figure 8.

![Figure 8. First principal stress (N/mm²) in the specimen for two consecutive increments of the finite element simulation of the partially healed specimen.](image)

In figure 8, the zones containing deactivated finite elements are shown in grey. It can be seen that these zones propagate, as the simulation progresses.

4. Conclusions

Various scenarios of the action of the healing agent on a specimen made of a cement-based composite and subjected to a quasi-static four-point-bending test, have been investigated numerically: a) a continuous action of the healing agent throughout the loading history and b) partial healing after a preloading phase and subsequent loading. The effect of the healing agent has been demonstrated in the finite element simulations. The mechanical behaviour of the specimens is characterized by the reaction force-deflection relationships.

The novelty of this paper is in the implementation of the Damage Mechanics based approach for modelling the mechanical response of structural members made of cement-based composite and subjected to self-healing.

Clearly, experimental validation of the numerical predictions is required. Moreover, an experimentally obtained input is needed for the better calibration of the material constants. In this context, the numerical investigation in the contribution focuses on a case study that can be, relatively easily, reproduced experimentally. The results of such characterization tests are required for the calibration of the damage-based model in its current form.

Further research work includes: (i) a mesh-sensitivity study, as a finer mesh will possibly provide more accurate results in terms of crack patterns obtained by finite element analysis; (ii) finite element modelling and simulation of various benchmark examples to validate the model for a broader range of geometries and load cases; (iii) investigation of the relationship between the crack width and the damage variable; study of the influence of these parameters and the effect of the healing agent on the mechanical response of a damaged structural member subjected to partial healing for practical purposes.
References

[1] Padture N P 2016 Advanced structural ceramics in aerospace propulsion *Natural Materials* 15 pp 804–9

[2] Mechtcherine V 2013 Novel cement-based composites for the strengthening and repair of concrete structures *Construction and Building Materials* 41 pp 365–73

[3] Yang H, Cui H, Tang W, Li Z, Han N, Xing F 2017 A critical review on research progress of graphene/cement based composites *Composites Part A: Applied Science and Manufacturing* 102 pp 273–96

[4] Ramasamy P, Stoica M, Ababei G, Lupu N and Eckert J 2020 Soft Ferromagnetic Bulk Metallic Glass with Potential Self-Healing Ability *Materials* 13 1319

[5] Norambuena-Contreras J, Arteaga-Perez L-E, Guadarrama-Lezama A Y, Briones R, Vivanco J F and Gonzalez-Torre I 2020 Microencapsulated Bio-Based Rejuvenators for the Self-Healing of Bituminous Materials *Materials* 13 1446

[6] Dry C M 1994 Matrix cracking repair and filling using active and passive modes for smart timed release of chemicals from fibers into cement matrices *Smart Materials and Structures* 3 pp 118–23

[7] Tittelboom K and Belie N 2013 Self-healing in cementitious materials – a review *Materials* 6 pp 2182–2217

[8] Ferrara L, Mullem T, Alonso M C, Antonaci P, Borg R P, Cuenca E, Jefferson A, Ng P L, Peled A, Roig-Flores M et al 2018 Experimental characterization of the self-healing capacity of cement based materials and its effects on the material performance: a state of the art report by COST Action SARCOS WG2 *Construction and Building Materials* 167 pp 115–42

[9] Mauludin L M and Oucif C 2019 Modeling of self-healing Concrete: a review *J. Applied Computational Mechanics* 5(3) pp 526–39

[10] Granger S, Piaudier-Cabot G and Loukili A 2007 Mechanical behavior of self-healed ultra-high performance concrete: from experimental evidence to modelling *Proc. 6th international conference on fracture mechanics of concrete and concrete structures, FraMCos-6*, ed Carpinteri A, Gambarova P G et al (London: Taylor & Francis)

[11] Hazelwood T, Jefferson A D, Lark R J and Gardner D R 2015 Numerical simulation of the long-term behaviour of a self-healing concrete beam vs standard reinforced concrete *Engineering Structures* 102 pp 176–88

[12] Mauludin L M, Zhuang X and Rabczuk T 2018 Computational modeling of fracture in encapsulation-based self-healing concrete using cohesive elements *Composite Structures* 196 pp 63–75

[13] Luzio G, Ferrara L and Krelani V 2018 Numerical modeling of mechanical regain due to self-healing in cement based composites *Cement and Concrete Composites* 86 pp 190–205

[14] Lemaitre J and Dasmorat R 2004 *Engineering Damage Mechanics: Ductile, Creep, Fatigue and Brittle Failures* (Berlin/Heidelberg: Springer)

[15] Mazars J J 1984 *Damage mechanics application to nonlinear response and failure behavior of structural concrete* Ph. D. Thesis (Paris: Paris 6 University)

[16] Mei J, Liu Z, Wen W and Sheng P 2007 Effective dynamic mass density of composites *Physical Review B* 76 134205