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MODELLING THE SELF-HEALING POTENTIAL OF DISSOLUBLE ENCAPSULATED CEMENT

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Abstract. In its fresh state, cementitious systems can be considered as colloidal suspensions build up from a mineral particles that follow a predefined grading. In this paper, a modelling approach that shows the healing potential of a blended cementitious system will be provided that consists of original cementitious particles mixed with so-called Dissoluble Encapsulated Particles (DEPs). DEPs are represented by a range of predefined fractions of original cementitious particles, but with its surface covered with a thin membrane. The self-healing principle of this system is based on the most basic healing process, where a delayed hydration of the DEP fractions may occur initiated by a crack. The crack actually triggers the membrane to open and exposes the still unhydrated DEP particles to water, after which the delayed hydration of the DEP system will take place, while closing the crack. The proposed model will demonstrate the healing potential of DEP inside a concrete and analyse the most dominant parameters affecting the mechanism. The membrane is considered to decapsulate by it's dissolution or cracking whenever being triggered by cementitious crack formation, which either lowers pH-conditions due increased CO_2 ingress, or induces mechanical stresses. The results show the potential of the healing mechanism to bridge a certain crack width, and shows, which fractions of a regular cement should be replaced in order the DEP system being most efficient. The numerical predictions also show that multi fraction DEP systems are more efficient then single fraction DEP, and that the addition of DEP does not affect the properties but may lead to a delay in the property development of cementitious systems.

1 INTRODUCTION

Many different ways that encourage the self-healing potential of cementitious materials have been developed over the last decades [1]. One of the methods that drives self-healing is by adding encapsulated containers filled with agents. These latter can be liberate whenever their containers (capsules) break, when hit by a crack. The disadvantage of this method is that often concrete incompatible materials are brought into the crack space. An alternative method close to this one is the so-called "Dissoluble Encapsulated Particles" (DEP) method [2] (Figure 1), where a number of predefined cement fractions are encapsulated by a membrane that dissolves whenever affected by a crack. Cementitious crack formation will trigger a DEP membrane to open due to 1) it's dissolution in lower pH-conditions due increased CO_2 ingress, or 2) due to induced mechanical stresses. The potential of this technique can be evaluated at different scale levels and at different time of age. In this, the initial quality of a cementitious microstructure will be the reference and complies with its predefined specifications. From this, the long-term durability performance, along with its initial quality, are the main parameters that determine whether self-healing materials are necessary and likely become activated during its service-life.

The self-healing potential of a concrete compatible agent might be necessary to maintain the microstructural quality of the initial material or to repair (micro)structural damages to reach an at least an even performance. The level of detail at which most common healing mechanisms occur, and at which they actively control the healing process most effectively, are the micro and nano-scale level. In this paper, emphasis will be on a preliminary modelling study that shows the potential of a self-healing cement, containing pre-encapsulated particles [3]. The micro-level modelling will demonstrate the healing potential of these so-called DEP-cements which are pre-blended with a predefined fraction of dissoluble encapsulated particles (DEP). The particles are activated at the moment that healing is required. This can be induced by cracking and/or by other damaging mutations of the internal microstructure, which also harm the encapsulation cover. In order to stay close to practice, the cement used for the modelling will be based on a standard Portland cement (CEM I), blended with an additional amount of embedded DEP-Portland one. With this research, the necessary conditions at which DEP cement performs well is investigated. The individual cement particles (DEP) are considered to be encapsulated by a fictitious viscous agent that acts as a membrane in high pH-conditions and opens (dissolves or cracks) whenever triggered by crack formation.

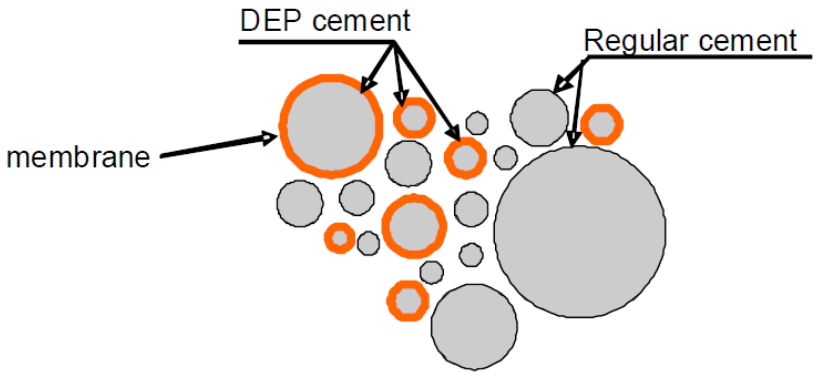


Figure 1: Schematic representation of regular cement blended with DEP cement [2]

Whenever the membrane dissolves after coming into contact with a crack, DEP cement will commence to react with the remaining capillary pore water or absorb it from the humid environment via moisture diffusion or transport through the cracks. The newly formed hydration products heal the damaged material.

2 MODELLING ENCAPSULATED PARTICLES

Modelling the encapsulated particles is achieved by creating a particle grading that has properties, which can be controlled explicitly during the hydration process. In this way a parameter study could be conducted showing the performance of the reacting DEP particles at later ages. For the hydration model, regular cement particles are blended with a predefined amount of DEP particles that follow a certain range of fractions and having defined hydrational properties. Therefore, focus of the model is on the different combinations of the encapsulated DEP particles, blended in a regular cement, and stacked randomly inside a virtual microstructure. Most effective combination in terms of cement and DEP fractions, in combination with the ability to close a crack will be analyzed. In this respect it is also relevant to know the ultimate crack width at which the healing mechanism will still work properly.

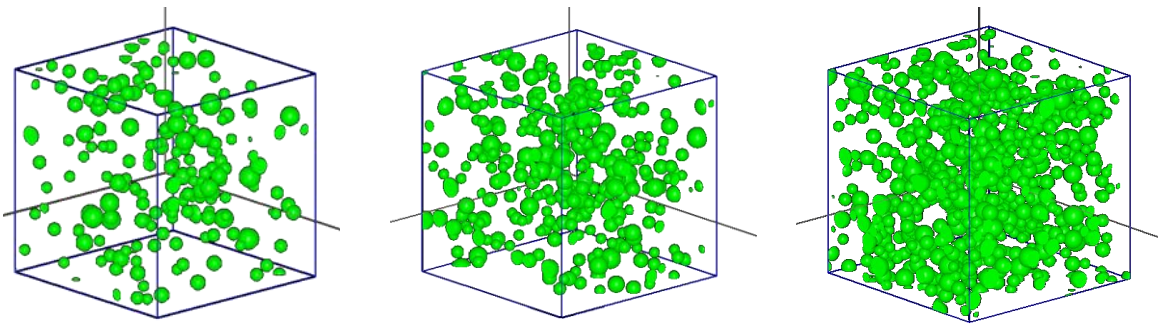
Therefore, regarding the numerical simulations, the following DEP combinations have been considered:

- 2.5%, 5% and 10% replacement of cement by DEP particles (see Figure 2);
- Replacement of the cement percentage is the same for all predefined fractions;
- The grading of DEP is equivalent to the grading of the cement;
- Particles are stacked randomly;
- The simulated volume is equal to 100 x 100 x 100 μm^3.

In order to get an impression of the replacement rates of the DEP particles in a cementitious system, Figure 2 shows random stacked particles at three different percentages. For this, the particles of both the original cement and the DEP fractions were placed according to the size distribution function of Rosin-Ramler (1) as follows

$$G(x) = (1 - \exp(b \cdot x^n) \tag{1}$$

being x the particle diameter, while n and b shape factors.



2,5% replacement 5% replacement 10% replacement

Figure 2: Impression of microstructures with displayed the 2.5%, 5% and 10% replacement of the regular cement by DEP inside a 100 x 100 x 100 μm^3 cube

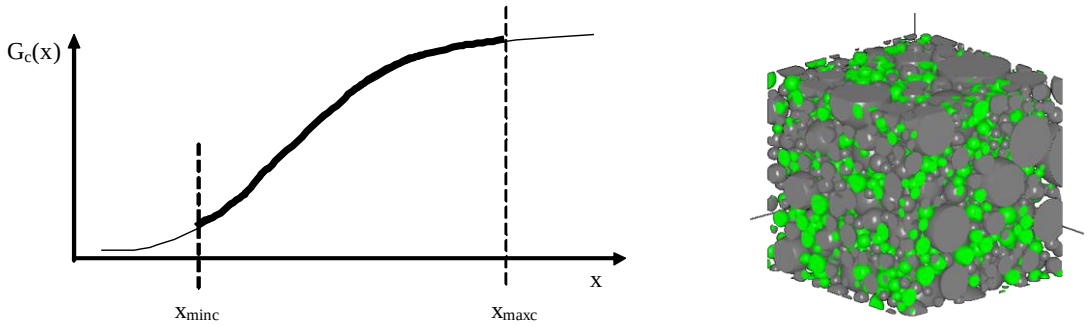


Figure 3: Left: Rosin-Ramler particle size distribution function for DEP and cement. Right: Blended initial microstructure with 10% DEP and 90% cement particles

This equation allows calculating the mass of each fraction that exceed a certain diameter. A schematic impression of the particle size distribution curve is shown in Figure 3 (left) and the initial result of the blended cement/DEP structure is shown in Figure 3 (right). The particle structure represents the starting point for the simulations conducted to determine most dominant parameters for the DEP self-healing mechanism. The encapsulated system will have their own reaction potential and are treated fully independently from the cement hydration. The hydration simulations are conducted with the Hymostruc [4] simulation model, which was developed at Delft University of Technology and is used to simulate the hardening process of the cement/DEP matrix. The Hymostruc model is a 3D code that can be used to simulate the hydration evolution of a virtual microstructure of cementitious materials. The model is based on a 3D scheme and calculates the development of the microstructure as a function of the particle size distribution, water-cement ratio, chemical composition and mix temperature for Portland and blended cement mixtures. The reaction kinetics of both cement and DEP granules are driving a particle expansion mechanism (Figure 4) that simulates the particle overlap and associated expansions of the surrounding C-S-H layers. The hydration process of the various particle reactions can be distinguished in different categories, including morphological, physical, chemical and thermo-dynamical issues. In view of the development of the cementitious microstructure, all these categories have their own particular characteristic and affect the hydration reaction in a certain way. This also holds for DEP particles, which will be in the main focus of the parameters that were changed during simulations.

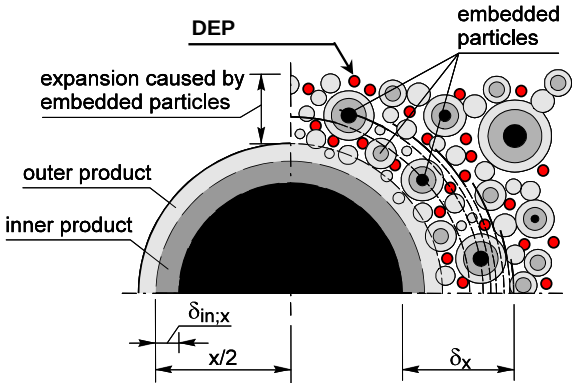


Figure 4: Schematic representation of expansion mechanism used in Hymostruc. The cement matrix is composed of hardening cement particles and unhydrated DEP grains. These will be activated after cracking and moistening

3 SIMULATIONS: MULTIPLE FRACTIONS APPROACH

Analyzing the potential of the microstructural model that was consisting of cement and DEPs, various grain configurations of cement/DEP blend were modelled and its hardening calculated. The basis of the model was based on adopting a microstructure with dimensions of 100 x 100 x 100 μm^3 (CEM I, w/c 0.45, Blaine 400 m^2/kg as shown in Figure 5). In the middle of this virtual microstructure, a crack (of 30 µm) has been initiated by means of shifting the initial randomly positioned particle to the left and right, while creating a void growth (crack) in the middle with a predefined thickness. This crack is the actual focus of this research and is influenced by the various parameter variations done in this numerical study.

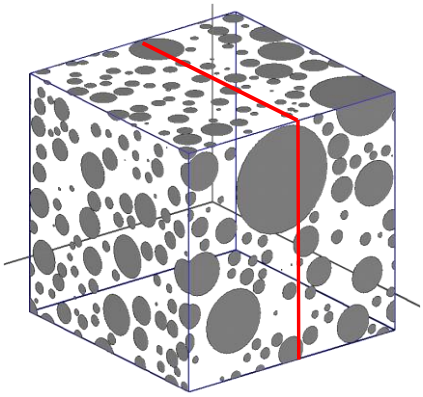


Figure 5: Schematic representation of the microstructure with the position of the crack in the middle indicated

The first parameter variation is on the replacement of a range of single fractions. In this so-called “multiple fractions approach”, 10% of the following cement fractions were replaced by DEP granulates, 5 - 10 µm, 10 - 20 µm, 20 - 30 µm and 30 - 40 µm. The grain structures of this cement and DEP matrices are shown in Figure 6. The microstructures give an impression of the partitions and DEP granules in the cement matrix and thus also give an indication of the geometric potential of the DEP granules in the matrix. The fine grains are the most abundant in number, but their expansion potential is relatively little. Larger grains are less abundant in number, but their expansion potential is much larger. What contributes most to the healing potential is analyzed hereafter and the optimum particle replacements are presented (Figure 7).

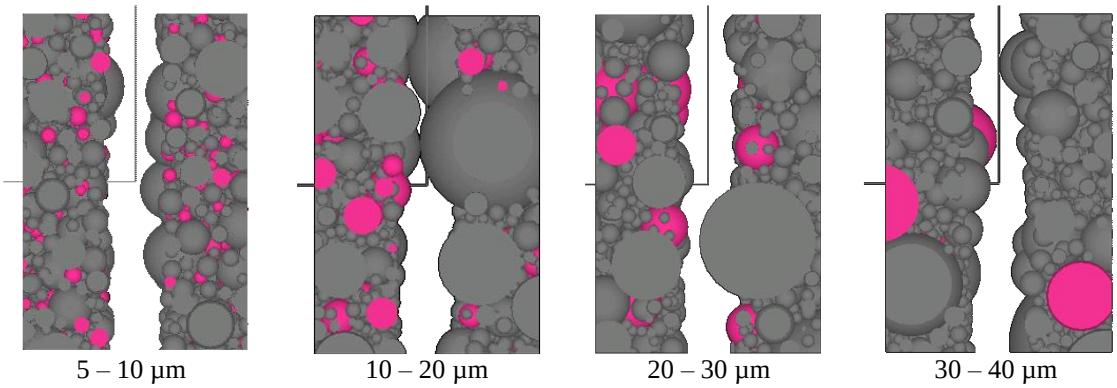
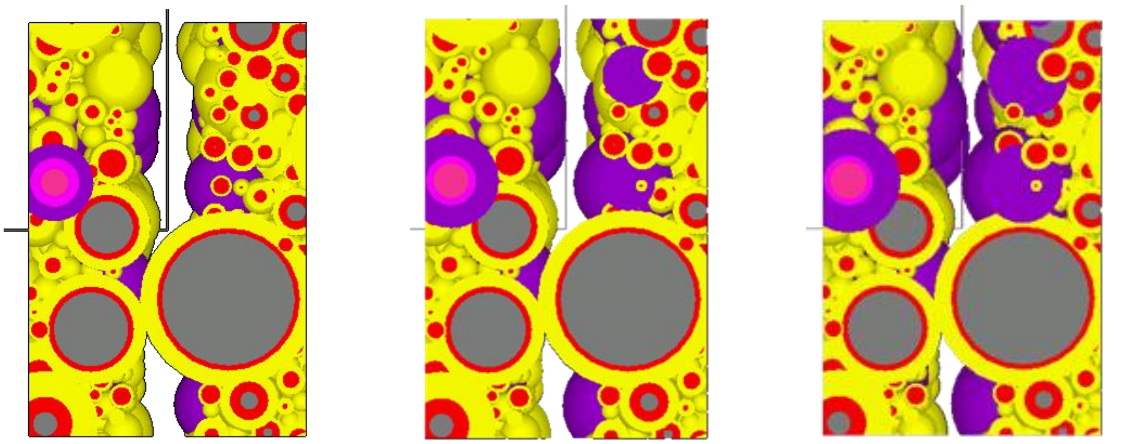


Figure 6: Multiple fractions approach: Initial state of microstructure by 10% cement replacement by DEP



Single fractions replacement:
10% DEP, 20 – 30 µm

10% DEP, 20 – 30 µm
DEP Expansion 2 x cement

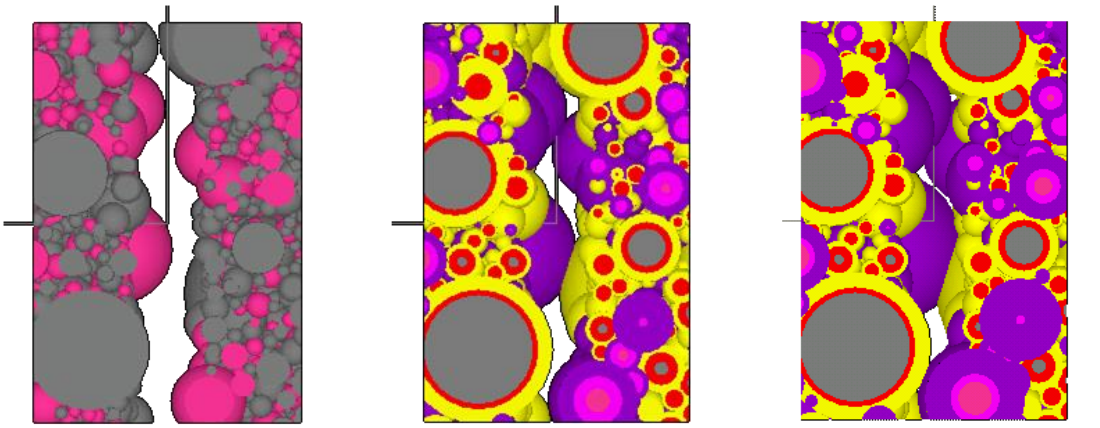
10% DEP, 20 – 30 µm
DEP Expansion 3 x cement

Figure 7: Single fractions approach (40 days.): left, 10% cement replacement by DEPs for the fractions 20 – 30 µm. Middle: same fractions replaced with double expansion of DEP particles. Right: same fractions replaced with three times the expansion potential. Hardening of cement and DEPs started at the same time

The simulations (duration 40 days) showed that, according to the multiple fractions approach, the optimum replacement range is 20 - 30 µm. The balance between the number of grains present in the system and the potential expansion appears to be the most optimal for this replacement range. Figure 7 (left) shows the healing potential of this particular blend, with the potential expansion of the DEP granules be equal to the expansion potential of cement. Figure 7 (middle), shows the simulation result of the same configuration with the DEP granules having an expansion potential of 2x the expansion potential of cement. From the results, it can be observed that the expansion potential has a relatively large influence on the healing potential. In Figure 7 (right), a simulation result is shown where the DEP granules expand 3x more than cement. These results show an even larger impact on the self-healing potential.

4 SIMULATIONS: ALL FRACTIONS APPROACH

In the “all fractions approach” a certain percentage of the full range of cement fractions is replaced by DEPs, representing the blended system. This replacement does not change the particle size distribution of the cement, but only differs in a way that a certain percentage of all cement fractions are encapsulated particles. This blended system represents the initial geometry of the granular structure and forms the basis for a microstructure with self-healing abilities. The chemical reaction of the cement particles will start right from the beginning while the DEP particles are considered to start after 28 days of cement hydration. With this, the DEPs will have the potential to add additional hydration products at a later stage whenever a crack appears. Activation of the DEPs, in the close vicinity of crack surfaces, will lead to a local solidification of the microstructure and to a reduction of the local capillary pore space [5,6]. The delayed formation of additional hydration products due to DEP reactions will be the main mechanism that drives the self-healing potential. In Figure 8, left, the initial situation of the blended system is shown, whereas the middle and right, shows similar and two times the cement expansions.



Replacement 30%, Crack width 30 µm

DEP expansion same as cement

DEP expansion two times as large as cement

Figure 8: Microstructure with 30 % replacement of cement particles by DEP with a crack width of 30 µm. Left, the initial state of the particle structure; middle, the initiated crack with a hydration of the initial particles up to 40 days and DEPs starting hydration after 28 days; right, similar with a double expansion potential of the DEPs

The degree of hydration of the blended system reflects the amount of binder (cement and/or DEP) that has reacted with respect to the original unreacted quantity. In Figure 9, the degree of hydration is shown as a function of the number of calculation steps of the Hymostruc model. This figure shows the following situations:

- "DEP activated at j=0", Cement and DEPs activated simultaneously at time t=0:
- "DEP activated at j=30", Cement activate at j=0, and DEPs activated at j=30 (=1000 hrs);
- "DEP particles"; DEPs are activated at j=30, which is 1000 hours after cement activation.

Figure 9 shows that the degree of hydration of the blended cement/DEP system has slightly reduced with respect to the initial situation where all particles react right from the start. The reason for this is that, until the DEPs are activated, they act as inert fillers in the microstructure.

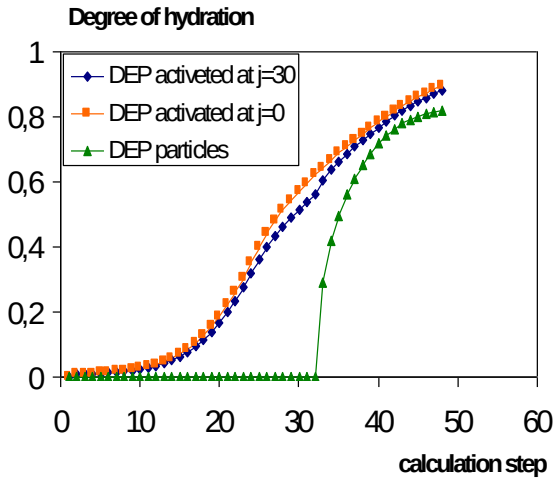


Figure 9: Degree of hydration versus calculation step of Hymostruc

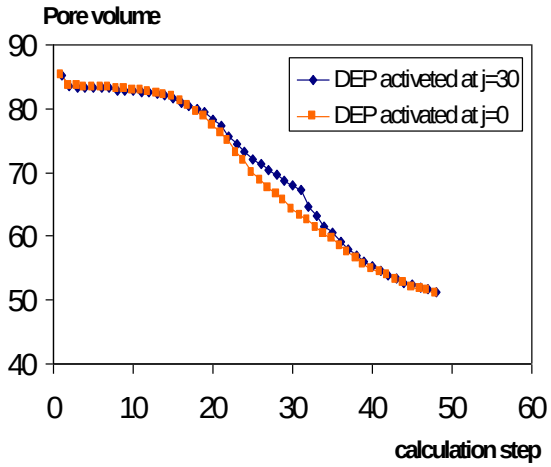
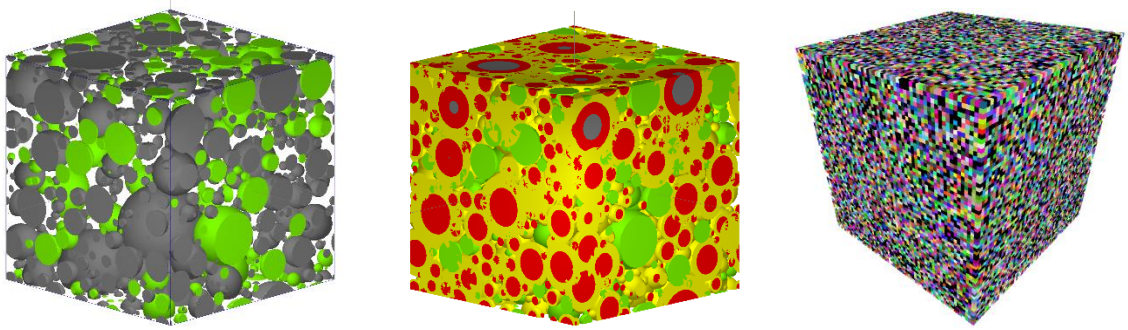


Figure 10: Development of capillary porosity for a system with and without the addition of DEPs

The question how the delayed DEP hydration affected the morphology of the microstructure can be evaluated whenever considering the porosity of the original and blended system. The porosity can be a measure for the strength of a cement based system and reflects also its durability. It is recalled that the addition of DEPs will initially or locally result in fewer hydration products being formed, which implicitly correspond to an increase in the local porosity of the blended system in comparison with the original cement matrix (without the addition of DEPs) [7]. Comparing these two systems will give an impression on the magnitude of this effect. Figure 10 shows the evolution of the capillary pores volume plotted against the calculation steps. For the cement system without the addition of DEPs, the pore volume is continuously decreasing, starting at 85% and reducing to a relative volume of 50%. It should be noted that the volume created by the 30 µm crack has not been taken into account. Whenever considering the system with the addition of DEPs, it can be observed that up to the moment that the DEPs become activated (j=30), the porosity is slightly higher, and once activated, the porosity approaches the porosity of the original cement system without the addition of DEPs [8]. However, it should be noted that the porosity shown in Figure 10 reflects the porosity of the adjacent microstructure, and not the porosity of the crack. This is would be an interesting extension of the model to see how the crack (porosity) reduces due to the protruding particles.

5 TOWARDS MICROSCALE VOXEL-BASED FEM FOR SELF-HEALING

The micro-mechanical behavior of the self-healing process has been evaluated numerically by analyzing a representative volume element (RVE) of the DEP-cement paste system. Since the main interest of this study was to investigate the effect of the fracture and cracking evolution affecting the DEPs, several 3D-microscale geometries are currently under investigation. The aim is to analyze different sizes and distributions of DEPs on both the mechanical and porosity modification due to self-healing. 3D virtual DEP-cement microstructures were generated by the Hymostruc hydration model, where the microgeometries and hydration process are based on several input parameters: e.g., particle size distribution of the (anhydrous) cement, type of binder, water-to-cement ratio, age, mix temperature and DEPs distribution (Figure 11a-b). Then, a structured voxel-mesh can be straightforwardly obtained as result of the microscale analysis (Figure 11c).



(a) (b) (c)

Figure 11: 3D microstructure: (a) initial anhydrous cement and DEPs, (b) hydrated structure and (c) schematic voxel-based FE mesh

The test specimens take into account mainly four (micro-) phases: (i) hydrated cement phase, (ii) unhydrated cement phase, (iii) DEPs and (iv) voids. For the fracture analysis, the phases (i) and (iii) mainly represent the "crackable" ones (being DEPs the weakest zone between them), while the (ii-) phase is mainly considered as a rigid body embedded in the system.

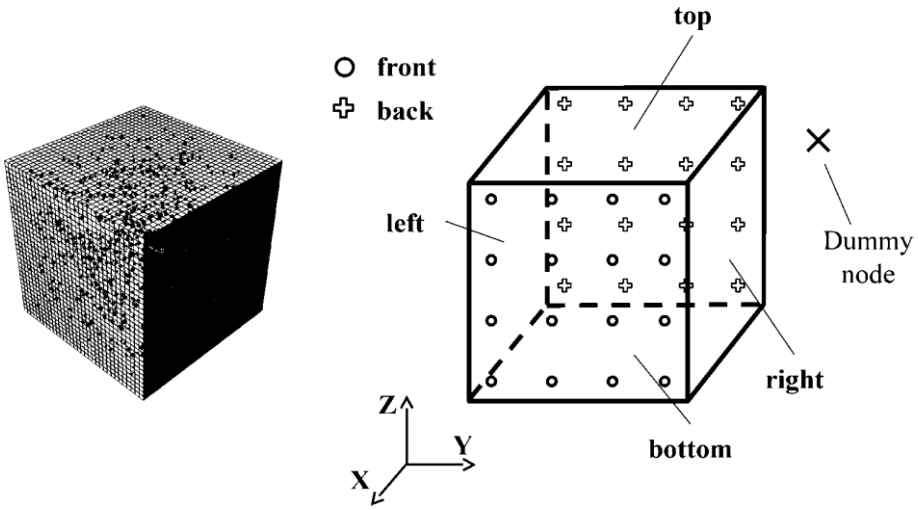


Figure 12: 3D RVE geometry (left) and general scheme of the boundary condition assumptions on the front/back and top/bottom surfaces

The numerical strategy thus tries to quantify the self-healing character of the DEPs by mechanically introducing cracks under general stress states. More specifically, in order to evaluate the self-healing capacity of the microscale specimens, three numerical steps will be sequentially considered into the micro-FEM analyses:

(i) in the **first stage**, the specimen was *"pre-cracked"* up to a certain level (namely residual crack opening level). At this stage, due to the imposed cracking, several DEPs will be broken and are able to develop self-healing mechanisms;

(ii) **Conditioning stage**: in this second step the self-healing processes develops. Hydration activities of DEPs aim at closing the fracture in the crack surface and also allow to consider possible mechanical recoveries and/or developments at the crack front.

(iii) **Final crack stage** which allows to evaluate the total failure of the specimen and with which it can evaluate the self-healing potential at a mechanical standpoint.

Periodic Boundary Conditions (PBCs) are used in the above cracking stages (i and iii). For this, the boundary domain Γ_μ of the (micro-)cubic geometry in Figure 12 is divided in two sub-domains outlining the opposite unit normals (surfaces). Due to the structured mesh, and in light of the PBC, each node with coordinates $\vec{x}^+$ in $\Gamma_\mu{}^+$ has a unique correspondent node $\vec{x}^-$ in $\Gamma_\mu{}^-$.

The cracking behavior is accounted for by means of the XFEM discontinuous-based technique [9]. One of the main advantages of this method is the (almost) mesh independency of the fracture propagation (when sufficiently refined meshes are employed) and there is no need to insert special interface (cracking) elements inside the voxel FE. In presence of a crack, additional DOFs enrich the nodes of the XFEM model, as shown in Figure 13.

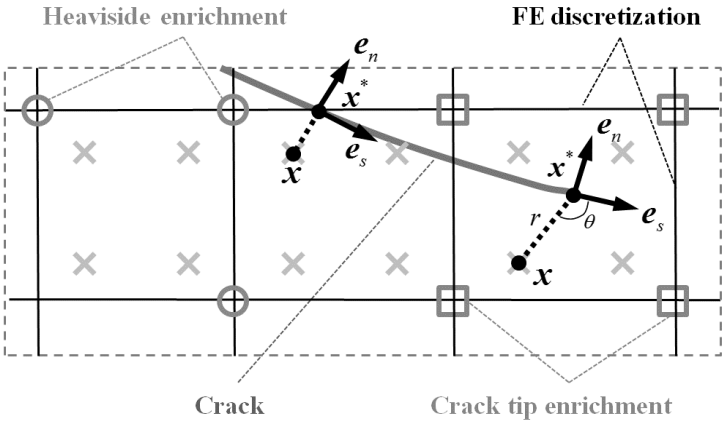


Figure 13: Enrichment of the nodes on the XFEM method employed in the voxel-based FE meshes

The so-called Level Set Method (LSM) [10] is used to locate the crack within the domain. In the XFEM-LSM formulation two functions are classically needed to define the crack position. In this work, however, a traction-separation cohesive rule, which also accounts for self-healing mechanisms, is utilized to model the crack initiation and growth along and arbitrary cracking path. This implies that cracks will propagate across an entire element at a time. This permits to avoid the need of modeling the stress singularity of the near-tip, and therefore, only the displacement jump across a cracked element is modelled [11].

To account for the degradation and potential failure of the involved elements, the traction-separation cohesive behavior is based on the interface constitutive theory for cementitious materials under possible self-healing effects as proposed in [6].

Table 1 shortly summarizes such proposal. The model deals with a damage-plasticity constitutive theory for zero-thickness interfaces and it is aimed at predicting time-dependent self-healing phenomena in cement-based composites. The material model is based on fracture-energy concepts and accounts for the time evolution of concrete porosity induced by the self-healing mechanism. A porosity-based model for self-healing phenomena and a continuous damage mechanics were also included in such proposal. Due to page limitations, many details are omitted in this work, however the complete discussion is available in [6] where the backgrounds of the modelling approached is extensively described.

Table 1: Overview of the interface model for self-healing effects in cement-based composites

	Fracture - based energy interface model for self-healing
Constitutive relationships	$\dot{\mathbf{u}} = \dot{\mathbf{u}}^{el} + \dot{\mathbf{u}}^{cr}$ $\dot{\mathbf{u}}^{el} = \mathbf{C_d}^{-1} \cdot \dot{\mathbf{t}}$ $\dot{\mathbf{t}} = \mathbf{C_d} \cdot \left(\dot{\mathbf{u}} - \dot{\mathbf{u}}^{cr} \right)$ $\dot{\mathbf{t}} = \left(\mathbf{I} - \mathbf{D} \right) \cdot \dot{\tilde{\mathbf{t}}}$
Yield condition	$f = \tilde{\sigma}_T^2 - (c - \tilde{\sigma}_N \tan\phi)^2 + (c - \chi \tan\phi)^2$
Flow rule	$\dot{\mathbf{u}}^{cr} = \dot{\lambda}\mathbf{m}$ $\mathbf{m} = \mathbf{A} \cdot \mathbf{n}$
Cracking work-evolution	$\dot{w}_{cr} = \tilde{\sigma}_N \cdot \dot{u}^{cr} + \tilde{\sigma}_T \cdot \dot{v}^{cr}$ $\quad \tilde{\sigma}_N \geq 0$ $\dot{w}_{cr} = \left[\tilde{\sigma}_T - \lvert \tilde{\sigma}_N \rvert tan(\phi) \right] \cdot \dot{v}^{cr}$ $\quad \tilde{\sigma}_N < 0$
Softening/re-hydration evolution law	$p_i = g_1\left(S[\xi_{p_i}]\right) g_2\left(\mathbf{SH}[\psi]\right) p_{0i}$
Isotropic damage	$d^{I/IIa} = \dfrac{e^{-\beta_d}\left(\dfrac{W_{cr}}{G_f^{I/IIa}}\right)^{\alpha_d}}{1 + (e^{-\beta_d} - 1)\left(\dfrac{W_{cr}}{G_f^{I/IIa}}\right)^{\alpha_d}}$
Kuhn - Tucker loading/unloading and consistency conditions	$\dot{\lambda} \geq 0, \quad f \leq 0, \ \dot{\lambda} f = 0$ **Kuhn-Tucker** $\dot{f} = 0$ **Consistency**

6 CONCLUSIONS

The model presented in this paper should be considered as a pathfinding approach to evaluate the potential of a self-healing mechanism that contains compatible cement particles with a delayed hydration ability, which is achieved by an (artificial) encapsulation material. The simulations are conducted with the Hymostruc model where the original cement particles as well as the DEPs are explicitly modelled. The results show that the potential of the model to calculate systems with unequal activation of the hardening reactions provides good insight in the cement hydration and porosity with and without DEPs.

Based on this conceptual approach, the following conclusions can be drawn:

- Blended DEP systems can be simulated well with hydration models such as Hymostruc;
- The particle grading and proportions of DEPs has a major influence on the healing potential;
- The all-fractions approach for the involved cement and DEPs indicated the larges healing potential;
- The degree of hydration of the blended cement - DEP system has the potential to develop to the similar level as the original cement hydration, after activation of the DEPs;

- The porosity of the blended cement - DEP system approached to the same level after activation of the DEPs compared to the original cement system.
- Voxel-based micro-structurers analyzed with XFEM could be a successful approach to model the breaking mechanisms triggering the self-healing behavior of DEPs.

7 ACKNOWLEDGEMENT

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