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RESEARCH PROGRESS ON NUMERICAL MODELS FOR SELF-HEALING CEMENTITIOUS MATERIALS

ABSTRACT

The paper discusses research progress on numerical models for self-healing cementitious materials (SHCMs). The paper considers models developed specifically for SHCMs, as well as other relevant work. This article provides a summary of current self-healing techniques along with descriptions of the processes that govern their behaviour. The paper discusses models for mechanical self-healing, transport processes in materials with embedded healing systems, fully coupled models and other modelling techniques used to simulate SH behaviour. The mechanics models discussed include those based on continuum-damage-healing mechanics (CDHM), micro-mechanics, as well as models that use discrete elements and particle methods. A considerable section is devoted to the simulation of carbonation in concrete since the essential mechanisms that govern this process are applicable to SH systems that employ calcite as a healing material. A number of transport models for simulating early-age self-healing are also considered. The paper highlights the fact that there are currently very few papers that describe fully-coupled models, although a number of approaches that couple some aspects of transport and mechanical healing behaviour are discussed. This article closes with a discussion that highlights the fact that many models have been presented with limited or no experimental validation.

1. INTRODUCTION

In a utopian world, structures would not crack , neither would they decay. This world is not utopia and present-day concrete structures do contain cracks and not infrequently decay to the point that they become unserviceable. The very nature of cementitious materials, which crack because they are relatively weak in tension, all-but precludes the development of a cost-effective crack-resistant concrete-like material. The next best scenario would be a cementitious composite material with in-built mechanisms for healing cracks as they form, such that any deleterious processes are halted before they cause significant harm. Cementitious materials do possess a natural ability to heal small cracks (Turner, 1937; Lauer and Slate, 1956; Edvardsen, 1999; Neville, 2002) but the state of many existing concrete structures shows that this mechanism is often insufficient to heal all cracks that form. Over the last decade, researchers have shown conclusively that it is possible to engineer self-repairing mechanisms into a cementitious composite material (Joseph et al., 2011; Wu et al., 2012; van Tittelboom and De Belie, 2013; Luhar and Gourav, 2015) to provide enhanced self-healing capabilities. Some of the healing techniques employed to-date aim to enhance natural 'autogenous' healing mechanisms (Ahn et al. 2010; van Tittelboom and De Belie, 2013; Lee et al., 2016; Gruyaert et al., 2016), whilst others are based on 'autonomic' -or manufactured- healing techniques (Dry, 1994; Jefferson et al., 2010; van Tittelboom and De Belie, 2013; Giannaros et al., 2016).

The potential benefits of self-healing cementitious materials (SHCM) are considerable. Their use would, in principle, dramatically reduce repair and maintenance costs in future structures. They would also increase the service life and effectiveness of structural repairs. These benefits have provided the motivation for a major research effort on SHCMs, which has been reported in an ever-expanding body of literature (Joseph et al., 2011; Jonkers, 2011; Wu et al., 2012; van Tittelboom and De Belie, 2013; de Rooij et al., 2013; Luhar and Gourav, 2015; Huang et al., 2016; Van Belleghem et al., 2017). The majority of this research has been experimentally based and, until recently, only a limited amount of work had been undertaken on developing numerical models for analysing these materials. This state of affairs has now changed such that there is a significant number of research articles on the simulation of SHCMs. It was therefore considered timely to write a state-of-the-art review on the numerical modelling of self-healing cementitious materials. In addition to reviewing

research directly on this topic, this article describes a number of other models that were not specifically developed for simulating cement-bound composites but that are considered relevant to the modelling of this class of material.

Before reviewing any numerical models, this paper first provides a very brief summary of SHCM technologies and relevant self-healing mechanisms. The review then continues by considering;

(i) models for mechanical healing;
(ii) the simulation of heat, moisture and chemical transport processes;
(iii) models for specific aspects of self-healing behaviour.

The review closes with a discussion and a few concluding remarks.

Before proceeding with Section 2, it is noted that this review is a product of a working group from the EU COST Action SARCOS (CA15202). This is one of three linked reviews, with the other two considering self-healing technologies and characterisation methods respectively (De Belie et al., 2018; Ferrara et al., 2018).

2. OVERVIEW OF EXISTING SELF-HEALING TECHNOLOGIES AND MECHANISMS

This section provides a very brief overview of existing self-healing technologies and mechanisms. Much more detailed reviews of past research on self-healing cementitious materials have been provided by others (Joseph et al., 2011; Wu et al., 2012; van Tittelboom and De Belie, 2013; Luhar and Gourav, 2015; Huang et al., 2016) and also will be provided by the linked SARCOS review papers referred to above.

2.1 Autogenous healing

Most researchers agree that there are three main mechanisms responsible for autogenous healing (Joseph et al., 2011; van Tittelboom and De Belie, 2013);

(i) continued hydration of unhydrated cement (Turner, 1937; Lauer and Slate, 1956; Neville, 2002; Granger et al., 2007; Huang and Ye, 2012.);
(ii) the formation of calcium hydroxide from the hydration of alite and belite and the subsequent formation of calcium carbonate from reactions between the calcium hydroxide and calcium carbonate (Lauer and Slate, 1956; Wagner, 1974; Edvardsen, 1999);
(iii) matrix swelling and crack 'clogging' by small particles bridging between crack surfaces (Clear, 1985; Edvardsen, 1999).

These mechanisms suggest that the degree of healing is highly dependent on the presence of water and unhydrated cement. This is supported by a number of experimental studies on autogenous healing that have shown that the degree of healing increases with the availability of water and the amount of unhydrated cement (Snoeck et al., 2014). Experimental investigations have also revealed that the amount of healing is a function of crack width (Edvardsen, 1999), with natural healing being unlikely to occur in cracks that are greater than 0.1mm in width (Edvardsen, 1999; Homma et al., 2009).

With regard to modelling, it may be concluded that a comprehensive model for autogenous self-healing needs to consider (i) the formation of cracks, including an accurate representation of the crack opening; (ii) a range of hydration reactions –in particular the formation of portlandite-; (iii) the flow (or transport) of water, heat and multiple chemical ions and; (iv) the mechanical healing of cracks via the three mechanisms described above.

The existence of these natural healing mechanism have encouraged researchers to find ways of enhancing autogenous processes and of trying to create conditions within the cementitious

composite that favour healing and self-sealing. One such technique involves the addition of capsules, or globules, containing superabsorbent polymers (Snoeck and De Belie, 2015; Lee et al., 2016), which ensure that a supply of water is available to aid the healing process. Other techniques, such as the inclusion of encapsulated sodium silicate within a cementitious mix, enhances the formation of natural cementitious products but may also be classed as 'autonomic' due to the manufactured nature of the supply system (Huang and Ye, 2011; Giannaros et al., 2016).

2.2 Autonomic healing

Alongside this work on autogenous healing has been a major research effort on autonomic (manufactured) healing systems (Joseph et al., 2011; Wu et al., 2012; van Tittelboom and De Belie, 2013; Luhar and Gourav, 2015). The three main techniques explored for delivering and releasing healing agents are;

(i) the embedment of brittle vessels (normally tubes) into structural elements (Dry, 1994; Mihashi et al., 2000; Joseph et al., 2010; Kanellopoulos et al., 2015);
(ii) the addition of microcapsules into cementitious mixes (Perez et al., 2015; Kanellopoulos et al., 2017) ;
(iii) the creation of interconnected channels or 'vascular networks' within cementitious structural members (Sangadji and Schlangen, 2012; Minnebo et al., 2017).

The range of healing agents encapsulated within these systems include single-component healing agents, such as cyanoacrylate, epoxy, and alkali-silica solutions, as well as multi-component methyl methacrylate and epoxy resins; however, difficulties over achieving adequate mixing have been reported for multi-component healing agents (Dry and McMillan, 1996; Toohey et al., 2009) .

A very different approach to healing involves incorporating shape memory material elements into cementitious structures. Shape memory alloy (SMA) bars (Kuang and Ou, 2008) have been shown to be effective at closing cracks in RC structures, although the cost of SMAs makes such a system unviable for all but the most specialist applications. A group at Cardiff have shown the potential of using Shape Memory Polymer (SMP) tendons to close cracks and enhance autogenous healing (Jefferson et al., 2010; Isaacs et al., 2013).

2.3 Microbial healing

The final category of self-healing technique considered involves the incorporation of calcite producing bacteria into cementitious composites (Jonkers and Schlangen, 2008; Jonkers, 2011).

The pioneers of this technology (Jonkers and Schlangen, 2008; Jonkers, 2011) have developed a system that involves adding two biochemical components to a concrete mix. The first component comprises bacterial spores mixed with the cement paste and the second –the biochemical agent- is incorporated in expanded clay capsules that are included in the concrete mix. When a crack forms, free water -a necessary ingredient- disperses the chemicals over the crack surface and activates the bacterial spores, which gradually fill the crack space with calcite.

Following this brief review of basic self-healing technologies, attention will be turned towards models for mechanical healing.

3. THE SIMULATION OF MECHANICAL SELF-HEALING

A significant number of models for mechanical self-healing are described within the framework of continuum damage-healing mechanics (CDHM). This framework is derived from the theory of continuum damage mechanics (CDM) and therefore a brief introduction is provided to CDM.

3.1 A brief overview of continuum damage mechanics theory

The theory assumes that there is an effective area of micro-cracks (A_ω) that intersect a representative plane of material of area (A). The relative damage area is then expressed as a ratio ($\omega = A_\omega/A$), which is equated to the loss of stiffness of the material normal to that plane. ω is termed 'the damage variable' and necessarily lies in the range zero to one (Lemaitre and Desmorat, 2005). When the damage is assumed to be isotropic, ω is a scalar variable and the resulting relationship between the stress tensor ($\boldsymbol{\sigma}$) and small strain tensor ($\boldsymbol{\varepsilon}$) is as follows:

$$\boldsymbol{\sigma} = \left(1-\omega\right)\ \mathbf{D}_e : \boldsymbol{\varepsilon} \tag{1}$$

in which $\mathbf{D}_e$ is the elasticity tensor.

A more general form of damage constitutive relationship (Lemaitre and Desmorat, 2005), shown in equation (2), uses fourth order damage and identity tensors, $\boldsymbol{\omega}$ and $\mathbf{I}^{4s}$ respectively.

$$\boldsymbol{\sigma} = \left(\mathbf{I}^{4s} - \boldsymbol{\omega}\right)\ \cdot \mathbf{D}_e : \boldsymbol{\varepsilon} \tag{2}$$

A number of researchers employ the concept of effective stress ($\bar{\boldsymbol{\sigma}}$), which represents the stress applied to undamaged component of material, as given by:

$$\bar{\boldsymbol{\sigma}} = \frac{\boldsymbol{\sigma}}{\left(1-\omega\right)} = \mathbf{D}_e : \boldsymbol{\varepsilon} \tag{3}$$

Models vary greatly in the way that damage evolution is computed. Many use thermo-dynamic variables derived from the Helmholtz (HH) (or related) energy potential (Ψ) (Lemaitre, 1985; Simo and Ju, 1987; Oliver et al., 2002), which is given by:

$$\Psi = \frac{1}{2}\left(1-\omega\right)\ \boldsymbol{\varepsilon} : \mathbf{D}_e : \boldsymbol{\varepsilon} \tag{4}$$

noting that equation (1) is recovered from $\partial\Psi/\partial\boldsymbol{\varepsilon}$ and that the material density (ρ) has been not been included in this non-standard definition of the HH potential.

The energy release rate, or driving force, which is used to drive damage in many models, is given by:

$$Y = -\frac{\partial\Psi}{\partial\omega} = \frac{1}{2}\boldsymbol{\varepsilon} : \mathbf{D}_e : \boldsymbol{\varepsilon} \tag{5}$$

Another essential component of a damage model is the damage loading function (or surface) that has been expressed in terms of effective (or standard) stresses, strains or thermodynamic driving forces, e.g.

$$F\left(\bar{\boldsymbol{\varepsilon}}, \kappa\right) = f\left(\bar{\boldsymbol{\varepsilon}}\right) - \kappa \tag{6}$$

where κ is a damage parameter used to govern the evolution of the damage variable i.e. $\omega(\kappa)$. The equations are sometimes arranged such that $\kappa = max(\ f\left(\bar{\boldsymbol{\sigma}}\right), \kappa_0)$, where κ_0 is the initial value of κ (de Borst et al., 2012).

A damage mechanics formulation also requires a set of loading/unloading conditions, normally expressed as ($\dot{F} \le 0 \quad ; \quad \dot{\kappa} \le 0 \quad ; \quad F\dot{\kappa} = 0$), which are often referred to as the Kuhn-Tucker conditions.

A few examples of widely referenced damage models include Mazars (1986; Simo and Ju (1987); Mazars and Pijaudier-Cabot (1989); Comi and Perego, (2001).

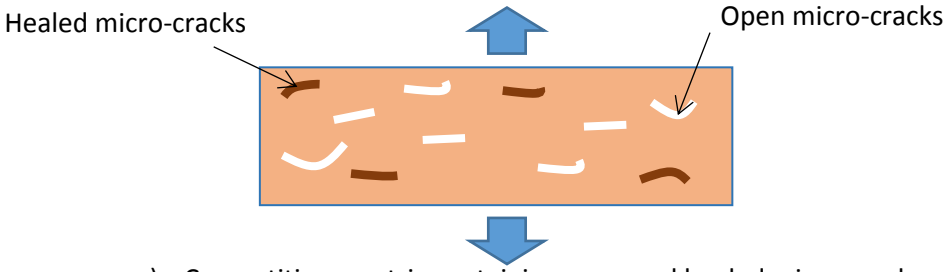
3.2 Models based on damage healing mechanics

Continuum damage mechanics provides a convenient basis from which to develop a model for damage-healing behaviour because CDM models have specific scalar or tensor variables that represent the effective loss of area due to micro-cracking, which can then be used directly in the simulation of healing.

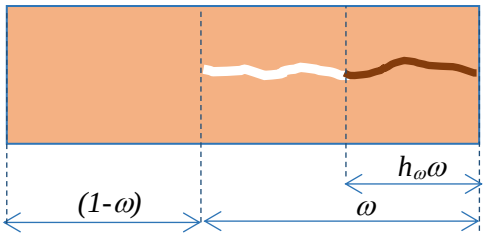
A generic stress-strain relationship for an isotropic CDHM, illustrated in Figure 1, is obtained by adding a healing term to equation (1), as follows;

$$\boldsymbol{\sigma} = \left(1-\omega\right)\,\mathbf{D}_e : \boldsymbol{\varepsilon} \;+\; h_\omega \cdot \omega \cdot \mathbf{D}_e : \left(\boldsymbol{\varepsilon} - \boldsymbol{\varepsilon}_h\right) \tag{7}$$

in which h_ω represents the portion of damaged material that has been healed and $\boldsymbol{\varepsilon}_h$ denotes a 'healing' strain, which would be associated with permanent strains derived from the healing process. As will be discussed below, $\boldsymbol{\varepsilon}_h$ (or equivalent terms) should be derived to ensure that thermodynamic consistency is maintained when material heals under non-zero strain conditions.



a) Cementitious matrix containing open and healed micro-cracks



b) Equivalent material representation showing proportions of undamaged (1-ω), damaged (ω) and healed material ($h_\omega\omega$)

Figure 1: Illustration of damage and healing components of a CDHM

A preliminary study on modelling self-healing was undertaken by Schimmel and Remmers (2006) (See also Remmers and de Borst, 2008) who developed a one-dimensional model to simulate idealised self-healing behaviour. The work involved the selection of a time-dependent healing function ($h_\omega(t) \in [0,1]$) and its insertion into a one-dimensional model that relates normal tractions (τ) to crack opening displacements (u). The model can reasonably be represented by the following 1-D form of equation (7):

$$\tau = (1-\omega)\, K u + (1-\omega_h)\, r\, h_\omega(t)\, \omega K (u - u_h) \quad (8)$$

in which K is an interface elastic stiffness term and r is a model parameter that defines the limit of healing.

The possibility of further damage occurring was addressed by the inclusion of the multiplier $(1-\omega_h)$ in the second term of equation (8), in which ω_h represents the proportion of healed material that re-damages. This preliminary work didn't include any validation against experimental data but did recognise many of the challenges involved in simulating damage-healing behaviour.

At a similar time, Barbero et al. (2005) presented a CDHM model for self-healing composite materials. In this work, the authors proposed a Helmholtz potential in terms of strains as well as damage, plastic and healing internal variables. The anisotropic damage and healing components of the model were based on the assumption that the principal directions coincided with the material axes of the composite and this resulted in a model with three independent damage and healing variables. The authors postulated the existence of a healing function that is the healing counterpart to the damage loading function. This idea was subsequently adopted by a number of other researchers. The authors of the present review question the usefulness of this approach and think that, in general, it makes more sense to compute healing from transport and curing phenomena. This is an important issue and is therefore revisited later in this review once other models that use this approach have been considered. Barbero et al. (2005) employed effective stress concepts in developing the plastic, damage and healing functions. They also describe a process for determining the healing parameters for the model that considers a shear test to failure and which gives the product of the damage and healing as the ratio between the virgin and ultimate shear modulus. Finally, the authors applied the model to the case of a composite carbon-epoxy material loaded in shear. No healing results were available at the time the work was undertaken so the authors calibrated their model using data from a no-healing material and then undertook a parametric study to demonstrate the effects of healing on the constitutive response of the material. The lack of healing results means that the accuracy of the model in a self-healing context system cannot be judged.

Neither the work of Schimmel and Remmers nor that of Barbero et al. was directed towards healing in cementitious composites but both of their modelling frameworks have relevance to such materials. By contrast, Granger et al. (2007) presented an experimental and numerical study on healing behaviour in ultra-high performance concrete (UHPC). The experimental investigation used notched prismatic specimens formed from UHPC, which were partially cracked in flexure and subsequently stored in water for different periods of time, to study the effect of curing duration on the degree of mechanical healing. The authors also presented 'a first approach of modelling', in which they developed a thermo-dynamic potential that included a healing term. The resulting one-dimensional constitutive equation, which relates uniaxial stress (σ) to uniaxial strain (ε), allows healed material to re-damage and may be expressed as follows:

$$\sigma = (1-\omega)\, E\, \varepsilon + (1-\omega_h)\, E_h(\Gamma_h)\, \varepsilon \quad (9)$$

in which E is Young's modulus and E_h is an effective Young's modulus of the healed material, which is a function of a curing parameter Γ_h.

The two damage variables (ω and ω_h) are assumed to depend upon the inelastic component of cracking opening across a crack-band (Bazant and Oh, 1983). It may be noted that no healing strain is included in the second right hand side term. This was not necessary for their simulations since the specimens modelled were unloaded during the curing phase; however, the authors themselves point to the limitations of this approach. In this model, $E_h(\Gamma_h)$ implicitly allows for the fact that only the damaged proportion of material is healed. Thus, if 100% healing was achieved and the healed material had the same stiffness as the new material, then the upper limit on $E_h(\Gamma_h)$ would be ωE. Some illustrative results from their work are presented in Figure 2, which shows experimental post-healing responses for two different healing periods. This shows that the model is able to represent the

post-healing response of these tests with reasonable accuracy but, as mentioned above, the model does not account for residual crack openings and thus cannot represent the full range of mechanical behaviour. Nevertheless, the formulation presented certainly made a valuable early contribution to the field.

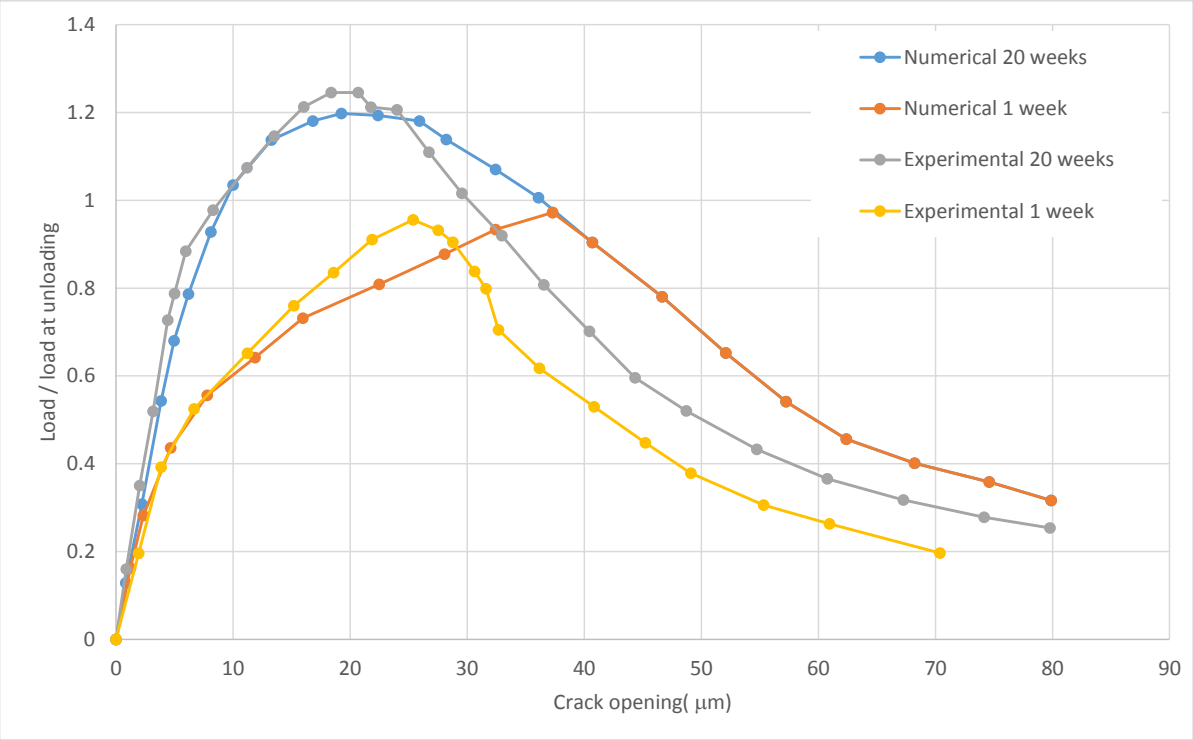


Figure 2: Illustration of results presented by Granger et al. (2007)

Mergheim and Steinmann (2013) directly addressed the question of the thermodynamic consistency of time-dependent healing under non-zero strain conditions. They assumed that healing starts immediately that damage takes place and that a healed increment of material is stress free upon formation, i.e., has a null increment of strain energy. It is the latter that ensures that spurious energy creation is not predicted. Their approach may be expressed as:

$$\boldsymbol{\sigma} = \left(1-\omega\right)\,\mathbf{D}_e : \boldsymbol{\varepsilon} \;+\; \left(1-\omega_h\right) \int_{s=0}^{s=t} \frac{\mathrm{d}h}{\mathrm{d}s} \cdot \mathbf{D}_e : \left(\boldsymbol{\varepsilon}(t) - \boldsymbol{\varepsilon}(s)\right) ds \tag{10}$$

in which h represents the relative proportion of healed material and s is a time variable.

The authors also allowed for healed material to be re-damaged (once) via the inclusion of the second damage parameter ω_h.

Another significant contribution in the work of Mergheim and Steinmann lies in their approach to time-dependent healing. They adopt a realistic exponential curing function, which is given below for an increment of healing material (h_i):

$$\Delta h_i = \Delta\omega_i \left(1 - e^{-\eta_h (t-s)}\right) \tag{11}$$

in which η_h is a curing parameter.

The authors then exploit the semi-group properties of such exponential functions to provide a convenient recursive update formula for the convolution integral. They subsequently present a parametric study undertaken with a 1D version of their model. This used the properties of a

thermoset material and investigated the response to a set of prescribed strain paths for a range of damage-healing cycles. No comparisons were made with experimental data that involved self-healing and thus we are not able to comment on the ability of the formulation to reproduce real measured behaviour; however; the results from the parametric study showed some interesting interactions between primary (virgin) damage, healing and re-damage.

Their healing evolution function could potentially be used for cementitious self-healing agents and linked to a transport model where the evolution rate would depend upon chemical concentrations. This model would need modifying to address the multiaxial micro-cracking response of a cementitious composite and would need extending to allow for the simulation of multiple damage-healing cycles and thermal effects. The work of Mergheim and Steinmann certainly goes beyond the previously mentioned contributions in that it provided a rational basis for simulating time dependent curing of healing agents.

An expansive plastic-damage-healing model framework was provided by Voyiadjis and co-workers (Voyiadjis et al., 2011 & 2012a, 2012b). The authors propose a thermo-dynamic (HH-type) potential that includes variables for isotropic and kinematic plasticity, damage and healing. The authors suggest new healing surfaces and couplings between damage, plastic (including visco-plastic) and healing model components. Voyiadjis et al. (2012a) also propose two new healing variables denoted h_v and h_v'. In this work, the primary healing variable (here denoted h_y) takes a value 0 for full healing and 1 for no healing, i.e. $h_v=1-h_\omega$. Their new effective healed modulus (in terms of a Young's modulus) is defined in two ways (i) with the assumption that the effective strain and the Cartesian small strain are the same and (ii) assuming an elastic energy equivalence. The latter leads to the following definition of the effective healing modulus ($\bar{E}_{hv}$):

$$\bar{E}_{hv} = E\left[\left(1-\omega\right)+\omega\left(1-h_v\right)\right]^2 = E\left[\left(1-\omega\right)+\omega\, h_\omega\right]^2 \tag{12}$$

noting that h_v corresponds to h in Voyiadjis et al. (2012a) whilst our definition of h_ω is used in the final expression in equation (12).

The new proposed healing variables are h_v (as above) and h_v', the latter of which is given by:

$$h_v' = \frac{\bar{E}_{hv} - E_\omega}{E_\omega} \tag{13}$$

in which $E_\omega = \left(1-\omega\right)E$

Voyiadjis and co-workers made the case that these variables are useful in characterising the physics of self-healing processes. Moreover, in Voyiadjis et al. (2012a), these healing variables are extended to address anisotropic damage-healing behaviour and, in this case, the scalar variables are replaced with 2nd order tensor variables.

In Voyiadjis et al. (2011 & 2012b), results from a set of one-dimensional simulations of tests on shape memory polymer specimens with self-healing capabilities are presented. These show that the framework is able to capture the main features of self-healing behaviour of a plastic self-healing composite.

The thermodynamic framework presented by Voyiadjis and co-workers could well be of relevance to SHCMs but considerable experimental and calibration work would be required to characterise the associated physical mechanisms and develop appropriate evolution functions for various forms of SCHM. It is the view of the current authors that starting the development of a model from a thermodynamic potential that contains many terms that are not used in subsequent examples makes it difficult to separate important from less important physical phenomena. Whilst we fully acknowledge that all models should satisfy the laws of thermodynamics, in our view, a better approach is to start by considering the important phenomena that need to be simulated in a self-

healing model, based on experimental evidence, and then developing a formulation that represents these phenomena.

In other work, Voyiadjis and Kattan (2014) discuss the idea of 'super-healing' materials that have healing recoveries greater than 100%. Experimentally, healing recoveries greater than 100% have been observed (Joseph et al., 2010) and such behaviour is attributed to the healed zone being stronger than the parent material but to our knowledge, no physical self-healing system approaches the level of super-healing discussed in this paper. Voyiadjis and Kattan (2017) furthered their investigations on CDH formulations by proposing a new logarithmic damage variable and providing definitions for 'damageability' and 'integrity'. These concepts are illustrated in Figure 3, which is redrawn from that in the original paper using the present notation. Time will tell whether these new variables are helpful in understanding and simulating self-healing behaviour.

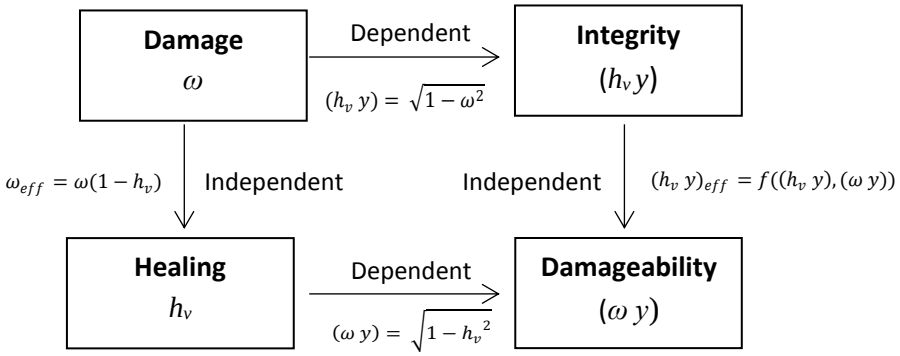


Figure 3. Damage, healing integrity and damageability concepts (Voyiadjis and Kattan, 2017)

Al-Rub and co-workers (Al-Rub et al., 2010; Darabi et al., 2012; Al-Rub, 2012a and 2012b) have developed a series of models aimed at simulating visco-plastic-damage-healing behaviour of asphaltic concrete. As with the work of Voyiadjis and co-workers, they adopted a thermodynamic potential as a basis for their model and defined various effective states used in the damage and healing evolution equations. In Darabi et al. (2012), the two effective states employed are those shown in Table 1 and the evolution of damage is driven by the stress in the 'healing configuration'.

Table 1. Effective states used by Darabi et al. (2012)

Nominal (or real) configuration	Healing configuration	Effective (undamaged) configuration
$\boldsymbol{\sigma}, E, A$	$\overset{=}{\boldsymbol{\sigma}}, \overset{=}{E}, \overset{=}{A}$ $\overset{=}{\boldsymbol{\sigma}} = \dfrac{\boldsymbol{\sigma}}{1-\omega\left(1-h_{\omega}\right)}$	$\overline{\boldsymbol{\sigma}}, \overline{E}, \overline{A}$ $\overline{\boldsymbol{\sigma}} = \overset{=}{\boldsymbol{\sigma}}\left[\dfrac{1-\omega\left(1-h_{\omega}\right)}{1-\omega}\right]$

The most comprehensive formulation in this series of papers is presented in Al-Rub et al. (2012a) which describes a model that is able to simulate the time, temperature, and rate-dependent behaviour of asphaltic concrete. Key features of the theory are a thermodynamic framework which includes the decomposition of the damage and healing into their energetic and dissipative components: the use of a power equivalence hypothesis to relate a nominal configuration to particular damage and healing configurations, and the inclusion of temperature effects on viscosity, damage, and healing, the latter via the influence of enthalpy changes on reaction rates. A second linked paper describes work in which the model was applied to the analysis of a set of asphaltic concrete test specimens (Al-Rub et al., 2012b). This involved the determination of a set of model parameters using a systematic parameter identification procedure. The model was then applied to the simulation of a series of experimental specimens, including uniaxial and triaxial time dependent tests on asphaltic concrete, as well as a case including cyclic loading. It was found that the model predictions reasonably captured the measured behaviour but in some cases there were significant discrepancies, particularly in the predicted creep-recovery at high temperature.

Alsheghri and Abu Al-Rub (2015, 2016) used the thermodynamic framework from Abu Al-Rub (2012a,b) and Darabi (2012) and adapted it for a cohesive zone elastic-damage-healing model. The cohesive crack healing model is based on the decomposition of the crack region into two parts, one representing undamaged material with the other simulating damaged and healing material components. The model assumes that the rate of healing is much greater than that of the damage process. The damage and healing variables are split into their normal and tangential components. A parametric study was reported that aimed to determine the effect of the various model parameters. The second of these two papers (Alsheghri and Abu Al-Rub, 2016) reports on the implementation of the model in a finite element code and gives the results of a series of analyses for a set of PMMA fracture-healing tests on PMMA specimens tested by Judd and Kausch (1979). The results from these numerical simulations are in generally good agreement with the experiment data. Shahsavari et al. (2016) developed a constitutive model for simulating damage-healing behaviour in concrete. In order to distinguish between tensile and compressive responses, the authors employed a spectral decomposition in a manner similar to that used in a number of previous damage models (Simo and Ju, 1987) and also used the effective and healed configurations proposed by Al-Rub and Darabi (2012a). Model predictions are compared with some experimental data from uniaxial tests for cases without healing. A parametric study is then presented that illustrates the effects of changing the healing parameters on the response of the self-healing concrete.

Pan et al. (2017) have presented a generic CDHM for self-healing systems that involves distributed micro-capsules. In this work, the effective states of Darabi et al. (2012) are employed in a model that considers plastic behaviour in addition to healing-damage responses. A healing function is postulated that is a quadratic function of the primary damage variable as well as a micro-capsule concentration parameter. A set of theoretical damage-healing problems are considered with the model that include 'cutting damage' in a cylindrical specimen, puncture damage in a plate and flexural damage in a beam. The simulations are not compared with any real damage-healing experimental data.

In a number of the contributions that employ effective stress concepts, it is not clear to the present authors how permanent strains (or relative-displacements), arising from healing that occurs when cracks are open, are included. We would expect to see permanent strains appearing in the relationship between the overall stress tensor and the effective stress tensor, the latter of which represents stress in the undamaged portion of material.

3.3 Micro and meso scale models using a range of numerical techniques

Mathematical material models based on Eshelbian micro-mechanics (Nemat Nasser and Hori, 2013) simulate the effects of inclusions and micro-cracks on the mechanical behaviour of composite materials. This approach is particularly well-suited to the simulation of the mechanical behaviour of SHCMs since it provides information on the relative degree of micro-cracking in different directions and on the effects of inclusions, such a micro-capsules.

This type of model has recently been applied to study the effects of adding spherical microcapsules into a cementitious composite on the mechanical and transport properties of the material (Li et al., 2016). Their research included an experimental programme of work in which the degree of water absorption of pre-cracked cementitious specimens containing micro-encapsulated healing agents was used as a measure of healing. The results showed that the model was able to reproduce the effects of increasing microcapsule volume on the elastic properties of the material with reasonable accuracy. Furthermore, it was shown that the proposed approach could provide a means of predicting the degree of healing.

Davies and Jefferson (2017) adopted a micro-mechanical framework in the development of their 3D model for SHCMs Healing was incorporated into the model using a solidification formulation that allowed for healing under both null and non-zero strain conditions. Specifically, healed micro-cracks were simulated as inclusions which were assumed to be stress-free at the moment of healing. The model allowed for micro-cracking of the healed inclusions but did not include any mechanism for simulating re-healing of these second stage micro-cracks

The model was validated using the authors' own data as well as data from tests undertaken by others. Results from a simulation of the '20 week' UHPC specimens tested by Granger et al. (2007) are given in Figure 4 (see, Davies, 2014). The model did not address time-dependent creep and was restricted to one re-damage (re-micro-cracking) event. It also is not able simulate crack closure effects, although these have been included in other micro-mechanical models developed by the same team in Cardiff.

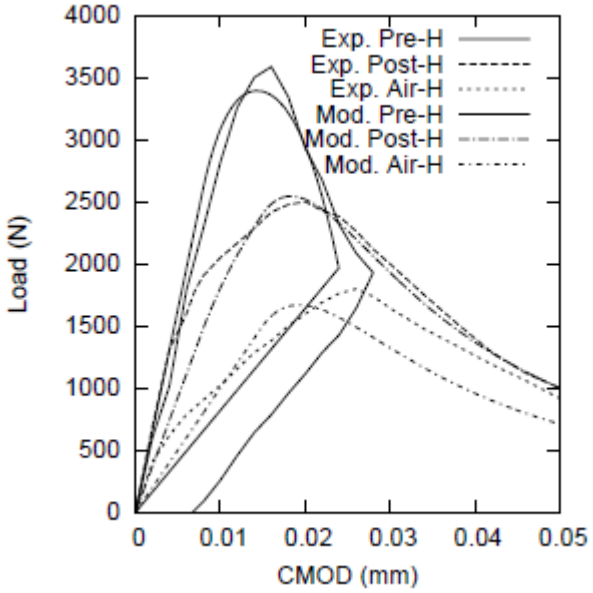


Figure 4. Simulation of the tests of Granger et al. (2007) (Based on Davies, 2014)

An analytical probability-based micro-mechanical approach has been taken by Zhu et al. (2015) to develop criteria for optimising microcapsule parameters with respect to self-healing behaviour. A simplified healing model is used and the parameters considered in their study include micro-capsule diameter and volume fraction of capsules in a mix.

Quayum et al. (2015) undertook some preliminary work on the application of homogenisation techniques to the evaluation the mechanical properties of self-healing concrete. In this work, the authors considered a number of homogenisation techniques, e.g. Mori-Tanaka-Voigt, and used the method to evaluate properties of cementitious matrices containing micro-capsules. The results from the homogenisation schemes were compared with those from a set of FE analyses in which the capsules were meshed explicitly. The authors concluded that care should be taken when applying linear homogenisation techniques to these materials and that further work and refinement is required on this approach

In a recent paper, Zhou et al. (2016) investigated the behaviour of a small crack adjacent to a circular void in a combined experimental/numerical study. The 'two-dimensional particle flow code' PF2D was used to simulate the specimens under increasing uniaxial compressive loading. The code was successfully validated using some experimental data and then the model was used in a parametric study that considered cracks of different lengths and orientations. The study showed that the final crack patterns and the way that micro-cracks coalesce between the pre-existing crack and the hole is also strongly influenced by both the length and orientation of the initial (pre-existing) crack. The study was seen as a step towards the development of a comprehensive 3D discrete element model of a SH material with multiple embedded micro-capsules.

The development of a 3D discrete model for microcapsule-enabled self-healing cementitious composite materials, referred to in Zhou et al. (2016), is reported in Zhou et al. (2017). In this work, the authors developed and implemented a new damage healing model in the discrete element code PFC3D. Their approach considers the healing derived from micro-capsules without explicitly modelling the capsules themselves. The model effectively simulates a continuum with a set of points that are linked by springs. A spring damage threshold is established and the spring released when this is exceeded. Healing is simulated by the reconnecting the points with a new spring that has properties which are derived from the healing system and a healing index defined in terms of the number of initial, healed and broken bonds (N_i, N_h and $\mathrm{N_d}$ respectively), as follows:

$$h = \left[\frac{N_h - N_d}{N_i - N_d} \right] \tag{14}$$

Using this model, the authors undertook a parametric study to explore the effect on the mechanical properties of the SH material of varying the strength and stiffness of the agent, the degree of damage present when healing occurs and the degree of healing. It was shown that the initial degree of damage and the strength of the healing agent both significantly influence the final strength of specimens after self-healing. The work constitutes a proof of concept and points to the potentially useful role that discrete element models could play in the development and evaluation of self-healing systems.

Caggiano et al. (2017) developed an interface model for simulating autogenous and enhanced self-healing in cementitious materials. Their model adopted an elasto-plastic-damage model framework with healing being introduced via the parameters that govern the evolution of the plastic-damage function. These parameters are made functions of a 'self-healing' porosity parameter that evolves with self-healing chemical reactions. The model predictions are compared with experimental data produced by Ferrara et al (2014). Two sets of experimental cementitious beams were considered, (i) which were made from a standard mix and were therefore subject to autogenous healing only and, (ii) beams made with a mix containing a crystalline admixture which was designed to enhance healing behaviour. The amount of self-healing in the experimental beams was relatively limited but the model showed that it could reproduce the experimental behaviour with reasonable accuracy.

Gilabert et al. (2017) developed a finite element model that used a combination of XFEM and the cohesive surfaces (CS) technique to simulate the mechanical behaviour of self-healing material systems with encapsulated healing agents. Two scenarios were explored; one was a micro-scale model that comprised a microcapsule embedded in a cementitious matrix and the other was a macro-scale model that considered the effect of adding tubular glass capsules on the overall bending response of a cementitious beam. The simulations were presented in detail and considered the manner by which capsules fracture as well as the effect of the capsules on the response of the structural member. One of the main findings of the work was that a minimum bond-matrix strength of 2MPa is required to ensure that a capsule breaks and releases its cargo. This conclusion applies to a typical 3mm diameter capsule with a thickness to diameter ratio of 0.06. The main stated aim of the work was to demonstrate that such models could be useful to experimentalists and those who develop self-healing systems.

A different approach to representing the meso-structure of particulate self-healing materials was taken by Herbst and Luding (2008), who used the Discrete Element method (DEM) to simulate healing in a material containing microcapsules. Their model considered load history dependency, elasto-plasticity, viscosity, adhesion and friction. Results were presented for a case with no healing, as well as for a scenario in which complete healing occurred instantaneously (i.e. all adhesion parameters were increased at the beginning of the simulation). It was shown that self-healing adhesion and the rate of damage detection both have a significant effect on the final strength and response of healed specimens. The authors recognised the need for time dependent healing where the strength slowly increases to mimic hardening of the healing agent and the need to allow for repeated healing.

Šavija et al. (2017) used lattice modelling to establish breakage criteria for a range of tubular polymeric capsules embedded in concrete. In the 2D lattice model used for the simulations, the cementitious matrix was represented by brittle beam elements whilst the capsules were modelled using beam elements governed by a multi-linear stress/strain relationship determined directly from experimental data. A nonlinear solution procedure was used to simulate a component of material subject to a prescribed uniaxial stress path under displacement control. The study showed that PMMA capsules with wall thicknesses of 0.3 and 0.7mm rupture when crossed by cracks of width 69μm and 128μm respectively. The work demonstrated that PMMA tubes with greater wall thicknesses and tubes formed from polyactic acid were unsuitable for this type of self-healing

application because they only ruptured when crossed by cracks which were much greater than 100 μm in width.

3.4 Discussion on mechanical models for self-healing cementitious materials.

No model is yet able to represent the entire range of mechanical behaviour observed in any type of self-healing cementitious material but the above review does suggest that models based on continuum damage-healing mechanics can reproduce some important aspects of this behaviour. We have doubts about the usefulness of some of the concepts employed in certain models, such as healing surfaces that are the counterpart to damage surfaces. It seems to us that it is more logical to simulate the transport of healing agents into cracks and then to simulate the curing of the agent in those cracks, allowing for the fact that the agent will cure in (an effective) stress-free condition. In this respect, we think that the model of Mergheim and Steinmann, although limited to 1D in their simulations, is particularly useful.

When more detailed representations of constitutive behaviour are required, models based on micro-mechanical behaviour are attractive because of their natural ability to represent anisotropic micro-cracking and healing under a wide-range of multi-axial stress-strain paths. Whilst promising, the models reviewed above are far from comprehensive and considerable future research will be required before they are suitable for large-scale simulations.

The models reviewed in the previous section on multiscale and particle-based methods -at present- look to be of most use in understanding the underlying mechanisms that govern the behaviour of SH materials and also show great potential in helping experimentalists design the components of SH materials e.g. properties of micro-capsules.

Having reviewed models for simulating the mechanical behaviour of self-healing cementitious materials, attention will now be turned towards models that describe transport processes in these materials.

4. MODELLING SELF-HEALING TRANSPORT PROCESSES

The technologies and underlying healing mechanisms discussed in Sections 1 and 2 of this paper highlighted the importance of chemical and fluid transport processes in many aspects of SHCMs. For example, the hydration reactions responsible for healing in early age concretes require the presence of anhydrous phases and water, both of which must be transported to a damage site prior to the occurrence of healing. On the other hand, carbonation reactions require portlandite, water and carbon dioxide. The classical mechanism for carbonation involves the ingress of CO2 through surface defects due to the material deterioration. Additionally, the consumption of portlandite during carbonation directly depends on the pH level within the cement matrix. This process generally leads to a pH reduction and an increased risk of reinforcement corrosion and associated loss of material durability (Papadakis et al., 1989; Papadakis et al., 1992; Bary and Sellier, 2004). This is a challenge for those developing self-healing materials that involve the production of calcite from the portlandite in a matrix.

A large number of models have been developed over the last few decades to simulate these processes accurately (Saetta et al., 1993, Saetta et al., 1995; Saetta, 2005; Bary and Sellier, 2004; Muntean et al., 2011), although only recently has the focus of this work been directed towards their predictive potential in the development of SHCMs (Zemskov et al., 2014; Aliko-Benítez et al., 2015). The remainder of this section reviews relevant research on transport processes. The main focus of this section is the transport processes and reaction kinetics associated with cementitious self-healing materials but for completeness some related and background work is considered. This starts with a short review of models for heat, fluid and chemical transport in porous media.

4.1 A brief overview of transport models in porous media

The majority of models dealing with transport phenomena in porous media are formulated within the hybrid mixture theory that makes use of macroscopic balance equations based on averaging techniques (Lewis and Schrefler, 1998). In this context, porous material is considered to be a multiphase medium where the voids in the solid skeleton are occupied by liquid and gaseous phases. Depending upon the temperature and the saturation degree, the liquid phase may consist of only bound water or also of capillary water (Gawin et al., 1999). Moreover, in the fluid phase there may also be dissolved (from precipitated crystals at the pore space) or leached (from the solid skeleton) chemical components (Gawin et al., 2008; Gawin et al., 2013; Chitez 2014; Chitez and Jefferson, 2015). The gaseous phase normally consists of a mixture of dry air and water vapour and is assumed to behave as an ideal gas.

The governing equations, at the macroscopic scale, are formulated in terms of averaged conservation equations for mass (of the different phases and chemical species), enthalpy and linear momentum balance under the assumption of local thermo-, hygral- and mechanical equilibrium (Gawin et al., 2006). For generality, non-specific sink/source terms are used in this introductory section (i.e. without making a distinction between hydration, leaching and/or precipitation processes). The equations - and relevant terms- will be presented for a deformable multiphase porous media, following the approach of Lewis and Schrefler (1998) and Gawin et al. (2003, 2006, 2013).

The volume averaged mass conservation equation of phase π is given by;

$$\frac{\partial \overline{\rho_\pi}}{\partial t} + div(\overline{\rho_\pi}\, \boldsymbol{v}^\pi) = \dot{m}_\pi, \tag{15}$$

where $\overline{\rho_\pi}$ denotes the phase-averaged density of phase π, $\boldsymbol{v}^\pi$ the velocity of phase π and $\dot{m}_\pi$ the net production of phase π. The term $\dot{m}_\pi$ may include components due to phase changes of water (evaporation/condensation, absorption/desorption, hydration/dehydration), chemical reactions and precipitation/dissolution of solutes, etc., and the effect of them on the heat balance. It is common practice (Lewis and Schrefler, 1998) to express the conservation equations in terms of the material time derivative referred to the solid phase, $\frac{D^s f}{Dt} = \frac{\partial f}{\partial t} + \nabla f \cdot \boldsymbol{v}^s$, where $\boldsymbol{v}^s$ denotes the velocity of the solid phase (, which for a deforming solid is given by $\boldsymbol{v}^s = \frac{\partial \boldsymbol{u}}{\partial t}$ with $\boldsymbol{u}$ the displacement vector). Then, the conservation equation (15) can also be expressed as:

$$\frac{D^s \overline{\rho_\pi}}{Dt} + div(\overline{\rho_\pi}\, \boldsymbol{v}^{\pi,s}) + \overline{\rho_\pi}\, div(\boldsymbol{v}^s) = \dot{m}_\pi, \tag{16}$$

where $\boldsymbol{v}^{\pi,s} = \boldsymbol{v}^\pi - \boldsymbol{v}^s$ denotes the relative velocity of the π phase with respect to the solid phase.

Developing the specific expression of the phase-averaged density $\overline{\rho_\pi}$ and decomposing the velocity $\boldsymbol{v}^\pi$ adequately, one can obtain the averaged mass balance equation for all the constitutive phases of the porous material in terms of the diffusive and advective fluxes, matrix deformation and the previously mentioned net production terms. Thus, we have the following mass conservation equations.

- For the liquid water phase: $\overline{\rho_w} = nS_w\rho^w$, where S_w denotes the pore saturation with the liquid phase and ρ^w denotes the density of the liquid phase. Then,
  $$\frac{D^s[nS_w\rho^w]}{Dt} + div(J_w^A) + nS_w\rho^w div(\boldsymbol{v}^s) = \dot{m}_w, \tag{17}$$
  where Darcy's law is used to compute the advective flux $J_w^A = \rho^w nS_w \boldsymbol{v}^{w,s}$.
- For the water vapour in the gas phase: $\overline{\rho_{gw}} = nS_g\rho^{gw}$, where S_g denotes the pore saturation with the gaseous phase and ρ^{gw} denotes the density of water vapour. Then,
  $$\frac{D^s[nS_g\rho^{gw}]}{Dt} + div\left(J_{gw}^D\right) + div\left(J_{gw}^A\right) + nS_g\rho^{gw} div(\boldsymbol{v}^s) = \dot{m}_{gw}, \tag{18}$$

where Fick's law is used to compute the diffusive flux $J_{gw}^{D} = nS_g\rho^{gw}\boldsymbol{u}^{gw,g}$ (with $\boldsymbol{u}^{gw,g} = \boldsymbol{v}^{gw} - \boldsymbol{v}^{g}$ denoting the macroscopic diffusive velocity of water vapour) and Darcy's law is used to compute the advective flux $J_{gw}^{A} = \rho^{gw}nS_g\boldsymbol{v}^{g,s}$.
Water evaporation appears as a sink term in $\dot{m}_w$ and a source term in $\dot{m}_{gw}$. Since no analytic expression is known for this term, equation (17) is frequently used as an evolution law for the mass change due to evaporation, $\dot{m}_{vap}$, and equations (17) and (18) are added to obtain a new equation independent of on $\dot{m}_{vap}$.

- For the solute x dissolved in the liquid phase: $\overline{\rho_x} = c_x nS_w\rho^w$, where c_x denotes the solute concentration per mass of pore solution. Then,
$$\frac{D^s[c_x nS_w\rho^w]}{Dt} + div(J_x^D) + div(J_x^A) + c_x nS_w\rho^w div(\boldsymbol{v}^s) = \dot{m}_x, \quad (19)$$
where Fick's law is used to compute the diffusive flux $J_x^D = c_x nS_w\rho^w\boldsymbol{u}^{x,l}$ (with $\boldsymbol{u}^{x,l} = \boldsymbol{v}^{x} - \boldsymbol{v}^{l}$ denoting the macroscopic diffusive velocity of the solute and $\boldsymbol{v}^l$ denoting liquid mixture velocity) and Darcy's law is used to compute the advective flux $J_x^A = c_x nS_w\rho^w\boldsymbol{v}^{l,s}$.
- For the dry air in the gas phase: $\overline{\rho_{ga}} = nS_g\rho^{ga}$, where ρ^{ga} denotes the density of dry air. Then,
$$\frac{D^s[nS_g\rho^{ga}]}{Dt} + div\left(J_{ga}^D\right) + div\left(J_{ga}^A\right) + nS_g\rho^{ga}div(\boldsymbol{v}^s) = \dot{m}_{ga}, \quad (20)$$
where Fick's law is used to compute the diffusive flux $J_{ga}^{D} = nS_g\rho^{ga}\boldsymbol{u}^{ga,g}$ (with $\boldsymbol{u}^{gw,g} = \boldsymbol{v}^{ga} - \boldsymbol{v}^{g}$ denoting the macroscopic diffusive velocity of dry air) and Darcy's law is used to compute the advective flux $J_{ga}^{A} = \rho^{ga}nS_g\boldsymbol{v}^{g,s}$.

A number of authors make simplifying assumptions with respect to the gas phase which negate the need for equation (20) to be solved explicitly (Bary et al., 2008; de Morais et al., 2009; Chitez and Jefferson, 2015).

The mass conservation equations previously presented are completed with the evolution laws for the mass source terms $\dot{m}_\pi$, full details of which may be found in Lewis and Schrefler (1998), Gawin et al. (1999, 2003, 2006, 2013), with a compact summary being given in Appendix A of Chitez and Jefferson (2015). The evolution of the porosity n is normally related to the time-dependent degree of hydration (Gawin et al., 2006). Following the principles established by Powers and Brownyard (1948), Chitez (2014) (see also Chitez and Jefferson, 2015) provided a specific link between the water consumed in hydration and the development of the pore structure within a cementitious matrix, thereby ensuring that the equation for porosity development was consistent with the moisture mass balance equation.

When porosity evolution is not considered explicitly, some authors use the solid phase conservation equation (21) to eliminate the derivative $\frac{D^s[n]}{Dt}$ from the previous conservation equations (Lewis and Schrefler, 1998).

$$\frac{D^s[(1-n)\rho^s]}{Dt} + (1-n)\rho^s div(\boldsymbol{v}^s) = \dot{m}_s \quad (21)$$

noting that $\overline{\rho_s} = (1-n)\rho^s$, where ρ^sdenotes the density of the solid material.

For non-isothermal cases, but under thermal equilibrium (i.e. same temperature for all phases), the volume-averaged enthalpy conservation equation reads (Gawin et al., 2013):

$$(\rho C_p)_{eff}\frac{D^sT}{Dt} + \left(\rho_w C_p^w\boldsymbol{v}^{w,s} + \rho_g C_p^g\boldsymbol{v}^{g,s}\right)\cdot grad(T) - div(\boldsymbol{J}_T^F) = \dot{m}_T, \quad (22)$$

where $(\rho C_p)_{eff} = (1-n)\rho^s C_p^s + nS_w\rho^w C_p^w + nS_g\rho^g C_p^g + c_x nS_w\rho^w C_p^x$ denotes the effective thermal capacity of the multiphase material, C_p^π the isobaric specific heat of phase π and $\boldsymbol{J}_T^F$ the heat flux given by Fourier's law.

In a fully coupled model, the system of governing equations would be completed with the conservation of linear momentum.

4.2 Self-healing by on-going hydration reactions

Due to the nature of hydration kinetics, models for early age autogeneous healing are based on a priori knowledge of the microstructure and composition of the cement paste. These are obtained as a function of the curing time from microstructural and stoichiometric models such as Hymostruc 3D (van Breugel, 1997) or STOICH_HC2 (Chitez 2014; Chitez and Jefferson, 2016), or by idealized representations (Lv and Chen, 2012).

The Hymostruc model (van Breugel, 1991; see also reviews in Chitez, 2014 and Cement science, 2012) was originally developed by a team at Delft University of Technology. In this model, cement particles are represented as spheres which gradually expand as the hydration process progresses. The primary assumption of the model is that new layers of hydration products are deposited on the surface of these spheres and when two of these spheres meet it is assumed that the further products develop around to two (now combined) spheres. The model simulates the development of properties of Portland cement, including the hydration process and the microstructure of the hardened cement paste.

The first work that used the Hymostruc model to represent self-healing in cementitious materials was undertaken by ter Heide (2005). In this work the author explored the effectiveness of the Hymostruc model to simulate autogenous healing. This work employed the bar and the ribbon models developed by Koenders (1997) and Lokhorst (1999). In their approach, clusters of hydration products were assumed to form as sets of horizontal bars which were linked by vertical elements.

A 3D version of Hymostruc was first developed by Koenders, which was later extended by Ye (2007) and one of the conclusions from their 3D simulations was that many cementitious materials have the potential to heal micro-cracks in specimens -or structural elements- that are up to twelve months old.

As discussed later in this section, Hymostruc was also used as a hydration model by Huang and Ye (2012). It was also further developed by Koenders (2012) (see below) and by its originator (van Breugel, 2016) who used the model to explore the filling of micro-cracks and the densification of the microstructure adjacent to cracks.

In general, hydration-based self-healing may assumed to be activated when moisture ingresses a structural element via a crack network, with the proviso that there is significant quantity of unhydrated cement within the element. To date, researchers have concentrated on simulating problems with one or more predefined cracks, although the issue of modelling healing in problems with evolving cracks –that make intersect unhydrated particles- has been addressed by Zemskov et al. (2011).

Koenders (2012) used Hymostruc to evaluate the potential of adding Dissoluble Encapsulated Particles (DEP) to a cementitious system which could later be activated by a crack and prevailing moisture conditions, while initiating a delayed hydration of the DEP particles with the aim to close the crack (Figure 5). The replacement degree was evaluated by replacing -for all fractions- the original cement particles by 10, 20 and 30% of DEP, following the same particle size distribution. The simulated volume was 100 x 100 x 100 μm^3. The simulations showed that a replacement of the cement particles over all fractions with the same percentage was most promising and could potentially close a crack with a width of 30 µm. In the study, the expansion potential of the DEPs was also varied, with one time having the similar outward growth of the C-S-H shell as the initial cement and another time with a twofold outward expansion of the C-S-H. The results are provided in Figure 6. It was observed that after 40 days of cement hydration, and activation of the DEPs after 28 days, the potential of DEPs available to act as a delayed source of cement for self-healing of cracks was sufficient. Koenders found that a critical factor in these kind of systems is the statistical distribution of the DEPs in relation to the crack and its potential to expand while depositing the hydration products in the crack to finally close it.

Koenders reported that various approaches had been taken to the evaluation of crack sealing potential through the addition of DEP grains. Several crack widths, particle size distributions and outward growth of the DEPs in relation to the cement particles of the microstructure were investigated. The multi-fractional blended system finally calculated had a 30% replacement and a fraction range corresponding to the fraction fragments of the cement. It was also found that after the hardening of the cement, the DEP grains began to cure to achieve a degree of hydration of 0.8. It also turned out that the porosity after activating the DEPs (28 days), and upon a certain period of time (≈40 days), the microstructure nearly regains the same value again as a cementitious system without DEPs. This implied that that the addition of DEP granules did not lead to a reduced porosity of the microstructure. The results of the study therefore led to the following conclusions:

- DEP systems can be modeled well with hydration models like Hymostruc;
- The grading of DEP grains has significant affect the healing potential of cement-DEP systems;
- The multi-fraction approach where the DEP grains have the same grading as the original cement has the greatest healing potential;
- The degree of hardening of a combined cement - DEP system may reach the same level as the original cement system;
- The porosity of a cement - DEP system reached a same level after activation of the DEP granules.

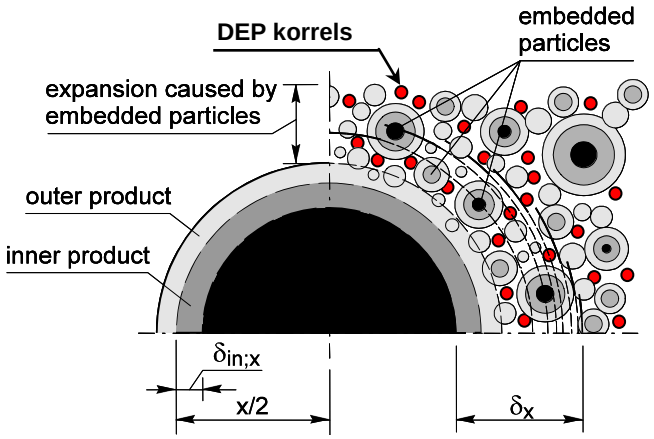
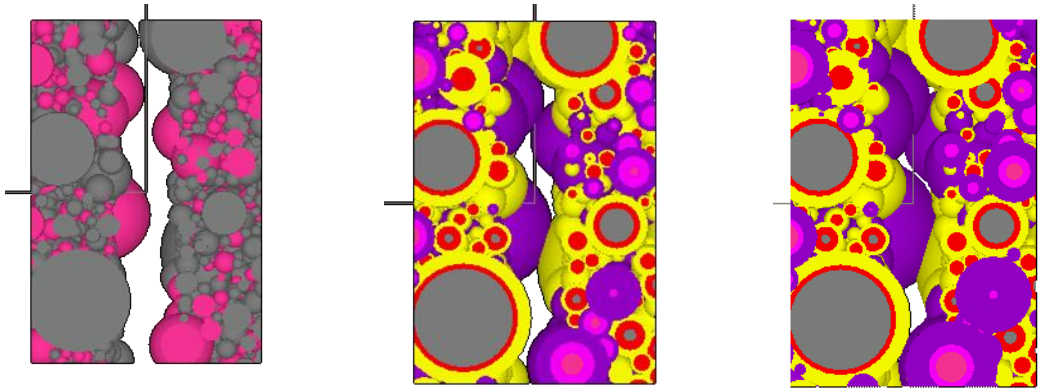


Figure 5: Schematic representation of the microstructure of a hardening cement grain by means of the grain expansion mechanism as used in Hymostruc. The cement matrix is composed of hardening cement particles and unhydrated DEP grains. These will be activated after cracking and moistening.



Replacement 30%, Crack width 30 µm

DEP expansion same as cement

DEP expansion two times as large as cement

Figure 6: 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 effect of moisture availability for the hydration reactions was analysed by Huang and Ye (2012). They formulated a hygro-electro-chemical model for the precipitation of hydration products in a predefined crack of 10μm width. The model considers the release of water from pre-mixed encapsulated reservoirs that are broken during cracking. Additionally, the fraction and distribution of unhydrated particles were obtained from Hymostruc 3D. The model takes into account the contributions from both CSH and CH phases, and is formulated using mass balance equations for moisture and ion concentration in the cement matrix, as well as ionic charge balance and thermodynamic equilibrium. The entry of carbon dioxide is blocked in the experimental set up, and hence calcite precipitation is not taken into account. The healing efficiency, defined as the volume ratio of newly formed hydration products and of the crack void, is computed over time and for various saturation conditions. In their model, the transport of ion *i* is simulated with a standard Fick's diffusion equation, as follows:

$$\frac{\partial C_i}{\partial t} = \nabla \cdot \left(D_i \nabla C_i \right) \tag{23}$$

The model also allows for changing diffusion properties within the crack zone as material is precipitated into the crack. This is accomplished using a linear interpolation between an initial diffusion coefficient ($D_{i,0}$) and that for the fully hydrated products ($D_{i,HP}$), i.e.;

$$D_i = D_{i,0} - \left(D_{i,0} - D_{i,HP} \right) \cdot n_s \tag{24}$$

in which n_s is the is the fraction of solid phases in the pixel-elements of water-filled cracks.

Their results indicated that stored water can be used to promote sustained hydration, although the newly formed precipitates may block the transport of ions and eventually inhibit further hydration. They concluded that the healing efficiency shows a linear dependency on the amount of released water, although two clearly distinct slopes were identified. This indicates that ahead of a certain threshold, the gain in healing efficiency is hindered due to the interaction between new hydration products.

Lv and Chen (2012) proposed a theoretical probabilistic model to assess the self-healing efficiency in Portland cement mixtures. The model is based on a Weibull distribution of the unhydrated cement particles, and two crack modes are considered: one in which the particles are broken by the crack, and other in which the crack circumvents the particles. The amount of material made available for the hydration reactions is different for each of the crack modes, and the self-healing efficiency was analytically addressed in terms of the volume of the produced hydration products.

Chitez and Jefferson (2016) (See also Chitez, 2014) developed a hygro-thermo-chemical model based on the theory of mixtures for porous media to simulate the healing of early-age Portland cements of different compositions. The model is formulated in terms of the conservation equations for water, the mass of unreacted cement and enthalpy, and takes into account different forms of water within the CSH gel, using the colloid model of Jennings (2008).

The balance equation (25) considers the net ionic concentration (ω) of reactive cementitious material.

$$\frac{D^s \overline{\rho}_\omega}{Dt} + div\left(J_\omega^A\right) + div\left(J_\omega^{DD}\right) = -\dot{m}_\omega \tag{25}$$

The source of ω is related to the amount of unhydrated cement and the precipitation of hydration products in a saturated crack is computed using a Freundlich type isotherm. The model also adopts the expression for the evolution of porosity given by Chitez (2014) (see also Chitez and Jefferson 2015). The STOICH_HC2 model is used to trace the formation and evolution of the porous network, and this takes into account the stoichiometry and hydration degree of the different unhydrated compounds. The predictions from an analysis of the 14-day samples of Huang et al (2013) are compared with the associated experimental results is given in Figure 7. Overall it may be stated that

the model predictions correlate quantitatively with experimental observations for different crack widths (from 10μm up to 188μm) and moisture conditions; however, this model does not consider the separate diffusion behaviour of ions within the solute and was not coupled to a model for the mechanical behaviour of the material. Never-the-less, it does represent a tractable method for simulating the transport processes associated with early age autogenous healing.

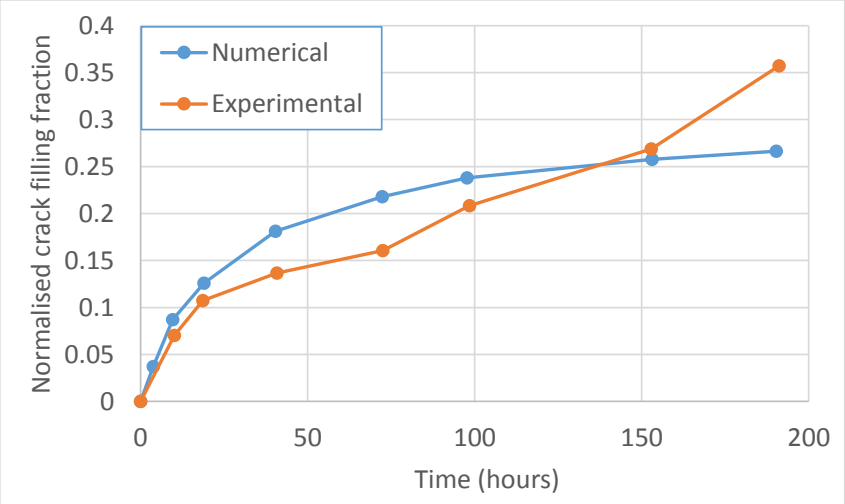


Figure 7. Plot showing a comparison between the experimental data of Huang et al (2013) and the self-healing model of Chitez and Jefferson (2016)

4.3 Self-healing by carbonation reactions

Carbonation is an autogenous self-healing mechanism of concrete in which aqueous carbon dioxide on the pore network reacts with several reactants to produce calcite. The main carbonation reaction, given in equation (26), may be attributed to presence of portlandite (Peter et al., 2008)

$$\mathrm{Ca(OH)_2(s \rightarrow aq) + CO_2(g \rightarrow aq) \rightarrow CaCO_3(aq \rightarrow s) + H_2O} \quad (26)$$

although hydration products such as calcium-silicate-hydrates (CSH) and unhydrated constituents such as tricalcium silicate (C_3S) and dicalcium silicate (C_2S) may also be involved in the production of calcite (Peter et al., 2008), as follows;

$$(3\mathrm{CaO} \cdot 2\mathrm{SiO_2} \cdot 3H_2O) + 3CO_2 \rightarrow (3\mathrm{CaO_3} \cdot 2\mathrm{SiO_2} \cdot 3\mathrm{H_2O}) \quad (27a)$$

$$(2\mathrm{CaO} \cdot \mathrm{SiO_2}) + 2CO_2 + m\mathrm{H_2O} \rightarrow (\mathrm{SiO_2} \cdot m\mathrm{H_2O}) + 2CaCO_3 \quad (27b)$$

$$(3\mathrm{CaO} \cdot \mathrm{SiO_2}) + 3CO_2 + m\mathrm{H_2O} \rightarrow (\mathrm{SiO_2} \cdot m\mathrm{H_2O}) + 3CaCO_3 \quad (27c)$$

The particular contribution of the latter product becomes relevant when the curing time is shortened.

The crucial role that carbonation reactions play in the durability of a concrete structure is not only related to the positive effects of autogenous self-healing but also to the negative effects associated with reinforcement corrosion. Corrosion is initially inhibited due to the high alkalinity of the cementitious matrix, which is related to the portlandite and CSH produced during hydration. As these phases are consumed during the different carbonation reactions, the solution pH decreases and the corrosion risk increases (Morenoa et al., 2004). Hence, an accurate prediction of the carbonation depth is of great interest and this has provided the motivation for the development of a number of mathematical models that simulate this process.

The two aspects of the carbonation reactions are evident in the literature. Earlier work (Papadakis et al., 1989; Saetta et al., 1993, 1995; Steffens et al., 2002; Meier et al., 2007; Peter et al., 2008; Muntean et al., 2011) focussed on the progress of the carbonation front to provide information regarding the

risk of reinforcement corrosion. However, more recent work (Zemskov et al., 2014; Aliko-Benítez et al., 2015) has examined the potential of natural and enhanced carbonation to heal microscopic cracks.

The idea of an advancing carbonation front was formulated by Papadakis et al. (1989). They developed a physicochemical model based on the diffusion kinetics of gaseous carbon dioxide in the pore network and its reaction kinetics with CH, CSH and unhydrated silicates. The authors made certain simplifying hypotheses, which included, one-dimensional axial symmetry and that no other reactions consume or produce hydration products; in addition, it was assumed that the position of the carbonation front over time could be analytically established. They concluded that the advance of the carbonation front is proportional to the square root of time (as in a Fickian diffusion process). They also established that the characteristic proportionality constant depends on the concrete composition at the end of the curing period (that is, the molar concentrations of the carbonatable species), the environmental conditions (that is, the molar concentration of carbon dioxide in gas phase) and the effective diffusivity of carbon dioxide in the pores of carbonated concrete. This effective diffusivity was measured under different conditions, and its strong dependency on the water-cement (w/c) ratio and water content was incorporated in the model. The analytical expression for the carbonation front was used to predict the carbonation depth in ordinary Portland cement in normal and accelerated carbonation test conditions for different w/c and w/a ratios, and validated against experimental data from their own laboratory and other laboratories. This model was further used to investigate the use of mortar coatings to prevent the inset of carbonation (Papadakis et al., 1992).

Saetta et al. (1993) proposed a hygro-thermo-chemical model for the spatio-temporal evolution of the CH carbonation reaction. The model assumes that hydration has been completed and calcium silicate hydrates are not present before the onset of carbonation. An Arrhenius equation is considered for the rate of the carbonation reaction, and the model incorporates phenomenological laws to attain the qualitative response of certain experimental observations. These include laws that describe the exothermic nature of the carbonation reaction, the consumption of carbon dioxide and the release of moisture resulting from the carbonation reaction, and the decrease of porosity due to the precipitation of calcium carbonate. The latter mechanism decreases permeability as well as diffusivities of both moisture and carbon dioxide. The model is used to predict the advance of carbonation on ordinary Portland cement of a fixed w/c ratio but subjected to differential environmental conditions, observing the delay of the carbonation progress at high relative humidity. The model was subsequently extended (Saetta et al., 1995) to analyse the corrosion risk of a reinforcing bar in the corner of a concrete structure subjected to periodical environmental conditions.

The seminal work of Saetta et al. (1993) has been considered and further extended by several authors. Steffens et al. (2002) extended the reaction kinetics proposed by Saetta et al. (1993) with a coupled temperature and moisture model. The carbonation rate is inferred from the amount of unreacted carbon dioxide, and the numerical predictions are validated against experimental results on OPC subjected to different curing times. Furthermore, the model is used to investigate the effect of environmental conditions on the carbonation depth of an L-shaped sample, quantifying the areas exposed to corrosion in both open and sheltered zones of the structure. Meier et al. (2007) considered a hygro-chemical carbonation model where the carbonation kinetics are defined through a power-law with a humidity dependent multiplier, and the matrix porosity evolves according to an exponentially decaying law that evolves according the carbonation kinetics. Henry's law is considered to include the effect of gas absorption, and exchange boundary conditions are considered at the exposed surface of the sample. The model predictions are compared with experimental results of natural and accelerated carbonation in ordinary Portland cements from Wierig (1984) and Papadakis et al. (1989) respectively. Peter et al. (2008) extended the work in Meier et al. (2008) to include CSH and CSH-producing unhydrated phases, in line with Saetta et al. (1989), to investigate the competition between the hydration and carbonation reactions.

In the work described above, the evolution of the carbonation front was tracked as a contour of an indicator species. In a different approach, Muntean et al. (2011) formulated a moving boundary problem for the portlandite carbonation process. In their model, the carbonated and uncarbonated regions are considered to be distinct (i.e. with different properties) and to evolve over time. Reaction-controlled interface kinetics govern the evolution of the interface (the carbonation front) separating these domains. This, more elaborated formulation of the problem, allows specific conservation equations to be considered for each domain, which include particularised matrix properties (as for example diffusion coefficients and gas absorption kinetics).

Carbonation has been also analysed as a self-healing mechanism. Aliko-Benítez et al. (2015) propose a physicochemical model for Engineered Cementitious Composite (ECC) materials (Li, 2003). Their model (illustrated in Figure 8) is based on the first order reaction kinetics of the dissociation reaction of calcite into its component ions (Ca^{2+} and CO_2^{3-}) in engineering cement composites. This three-species chemical model takes into account the diffusive transport of anions through the cement matrix, supplied into the material through on the external faces (the others being sealed) whereas cations are non-mobile, and the precipitation to solid calcite is taken to be instantaneous and governed by the following equation:

$$\left[\dot{\mathrm{CaCO}}_3\right] = k\left[\mathrm{CO}_3^{2-}\right] \cdot H\left[\mathrm{Ca}^{2+}\right] \tag{28}$$

in which the square bracket denotes concentration, k is a reaction constant and H is a heaviside function.

The model was built on the assumption that moisture and carbon dioxide are fully available in the cement matrix during the whole simulation period, and hence the carbonation reaction is sustained until the mass of cations is depleted. Damage, in the spirit of continuum damage models, was introduced as an internal variable and healing efficiency is defined as the ratio of the volume of newly deposited calcite precipitates and the prescribed volume of damage. Simulations on an idealised test problem allowed the healing efficiency to be computed as a function of damage, showing that the amount of damage that can be recovered over a fixed period of time strongly depends on anion diffusion and reaction parameters. For example, in a period of 30 days, complete healing is only attained for damages up to 0.4 (volume fraction) and for the range of fast diffusion and reaction. The potential of the model was also illustrated in the analysis of a three-dimensional T-beam specimen.

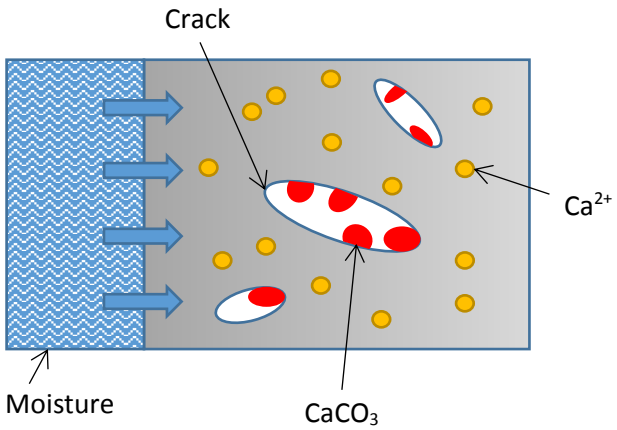


Figure 8. Diffusion mechanism of CO2 enriched moisture and CaCO3 precipitation in cracks. (illustration of the model of Aliko-Benítez et al., 2015)

The contribution of Aliko-Benitez et al (2015) was certainly more detailed in its treatment of the transport of chemical ions and the chemistry of the precipitation of healing products than the work of Chitez and Jefferson (2016). It is a pity that the former contribution didn't include any comparisons

with experimental self-healing tests that would have allowed a reader to judge the accuracy of the model in this regard. Nevertheless, the present authors believe that coupling the stoichiometric approach of Chitez and Jefferson, with the calcium transport and calcite precipitation formulation of Aliko-Benitez et al (2015) would result in a model that could simulate both short and long term autogenous self-healing processes with good accuracy.

Zemskov et al. (2014) also addressed calcite carbonation in the context of bacterial-based self-healing. The model considers the interplay of encapsulated compounds with a density of bacteria dispersed along the matrix. The model includes the dissolution of the capsule and the deposition of the calcite as moving interfaces, where the front velocities are derived from mass balance arguments. The model assumes full availability of oxygen and water within the matrix, where the capsule compounds (calcium lactate, sodium glutamate and monopotassium phosphate) diffuse and are consumed for the growth of the bacteria density through a Monod model. The model focuses on the contribution of a single capsule, and a sensitivity analysis on the capsule radius and crack width is provided. Moreover, taking into account the growth of the calcite phase in the crack direction, the effect of neighbouring capsules can also be inferred. As an example, the model is used to reveal that a crack width of 1 mm can be successfully healed with capsules of 1mm of radius and about 3mm of distance between capsules centres.

5. SPECIFIC ASPECTS OF MODELLING SELF-HEALING BEHAVIOUR

The natural extension to Sections 3 and 4 of this paper would be a review of fully-coupled models for mechanical and transport behaviour; however, to date, very little work has been carried out on such coupled models. This section is therefore devoted to a range of models and model components that don't fall neatly within the categories of work reviewed in Sections 3 and 4.

5.1 Coupled chemical hydration-mechanical models

Hilloulin et al. (2016) undertook a combined experimental/numerical investigation into natural healing of small cracks (5 to 20 µm) in cementitious specimens. In the numerical component of the work, the microstructural hydration model CEMHYD3D (or CEMPP) was combined with the finite element code Cast3M to simulate healing processes due to hydration. The cementitious micro-structure was discretised in CEMPP with particles of size 1 µm for a volume with characteristic dimension 100 µm. The hydration process was simulated via cycles of dissolution, diffusion and reaction, according to a known set of selected reaction equations. In order to study the mechanical regains due to healing, micromechanical tensile tests were performed on 3D subparts of the output microstructure. Finite element simulations were carried out on 20 × 30 × 10 voxels volumes for 5-µm wide cracks, or 20 × 30 × 15 voxels volumes for 10-µm wide cracks. Young's moduli of the small volumes were successively calculated using the CEMPP results for directions normal and perpendicular to the imposed crack (space). These time-varying elastic properties were to compute strength and stiffness regains due to hydration. An overall conclusion from the work was that very significant regains in mechanical strength and stiffness can be obtained within 2 weeks of casting, for cracks of width up to 10 µm.

di Luzio et al. (2017) extended the MM (Solidification-MiTextcroprestress-Microplane model M4) model (di Luzio and Cusatis, 2009 a,b 2013) to incorporate self-healing effects and, in particular, the effect of delayed cement hydration, which is the main cause of the self-healing in young concrete. These self-healing effects were taken into account by introducing an internal variable which characterizes the self-healing process, the effects of cracking on the diffusivity, and the positive recovering effect of the self-healing on the mechanical properties. The models were satisfactorily validated against the experimental results of Ferrara et al. (2014)

5.2 Simulation of embedded micro-capsules, capsule breakage and water release

Using results from Hymostruc3D simulations, Huang and Ye (2016) determined a relationship between healing efficiency and the amount of water released from broken capsules. In this investigation the authors also undertook a numerical investigation into the probability of a crack intersecting a microcapsule for a given distribution of micro-capsules. The study involved 1000 numerical experiments using different random distributions of particles. An approximate representation of their results is given in figure 9.

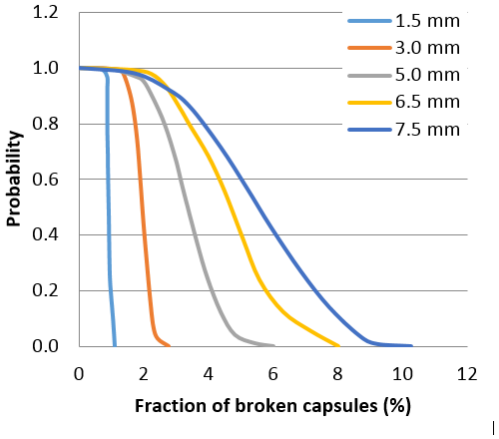


Figure 9. Probability of a crack hitting capsules with different sizes (5% capsule dosage) (based on the results of Huang and Ye, 2016)

The paper of Huang and Ye (2016) also reports on a study on the effect of including micro-capsules on the mechanical properties of cementitious matrices, which was undertaken using a lattice model (Schlangen and van Mier, 1992). They found that the rate of reduction in the elastic modulus, with increasing volumetric content of micro-capsules, was less than that of the tensile strength e.g. 7% volume of microcapsules results in a 17% reduction in the elastic modulus but a 50% reduction in the tensile strength. As a consequence of their findings, the authors recommended that the negative effects of adding capsules into a mix '*should be taken into account while designing the mixture of cementitious materials with self-healing capacity*'.

5.3 Models for permeability and the flow of SH agents

Liu et al. (2017) undertook a mainly experimental investigation into the the permeability properties of ECC under different degrees of micro-cracking. As part of this work they developed an analytical model to predict the permeability of ECC composites for different degrees of damage and self-healing.

The specific issue of simulating the flow of healing agents in natural cracks has been considered in detail by Gardner et al. (2012, 2014, 2017). Their investigations have explored the flow properties of a range of healing agents in artificial and natural cracks over a range of crack openings. The model developed by the authors is based on modified Lucas-Washburn equation and allows for stick-slip, meniscus and wall friction effects. The fluids considered include plain water, water with ggbs and pfa in suspension and cyanoacrylate. An illustrative result is given in Figure 10 for the capillary rise response of cyanoacrylate in an inclined planar crack in concrete. This level of agreement is representative of the model of Gardner et al, which suggests that their model could be used to predict such behaviour with a reasonable level of confidence.

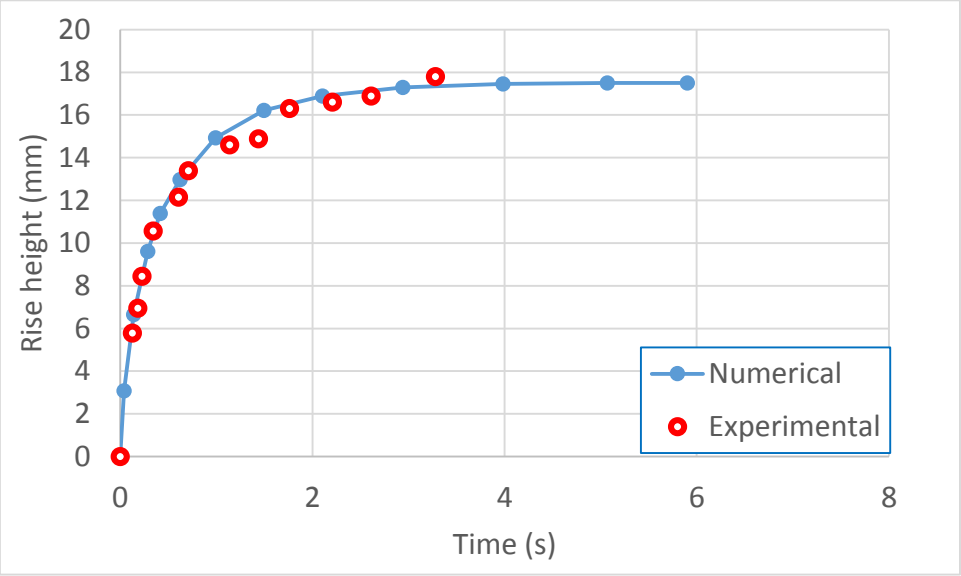


Figure 10. Comparison between experimental and numerical data of Gardner et al. (2014)

5.4 Simulating a SH system that uses Shape Memory Polymer (SMP) Tendons

Some modelling work has been undertaken on self-healing systems that employ SMP tendons to close cracks. This has included the development of thermo-mechanical rheological models for SMP tendons (Dunn et al., 2011, Hazelwood et al., 2015), as well as a layered beam finite element model (Hazelwood et al., 2015) for the simulation of cementitious beams in which SMP tendons have been embedded. The latter model allows for hydration, creep and shrinkage in the cementitious matrix, in addition to the thermo-mechanical behaviour of the SMP tendons. This type of self-healing system may be regarded as delayed prestressing and is therefore quite different in nature from the other systems considered in this review.

5.5 Nano-scale models

One aspect of modelling and experimentation that has not yet been considered in this review is nano-engineering but this is rapidly emerging field that could be highly relevant and beneficial to the development of SHCMs. The field encompasses techniques for manipulating material structures at the nanometer scale and potentially tailoring cementitious composites with superior properties and self-healing capabilities (Scrivener, 2009; Sobolev and Sanchez, 2010; Lushnikova and Zaoui, 2017; Sekkal and Zaoui, 2017).

Research undertaken to-date has shown that understanding and modifying the structure of C-S-H at the atomic level could be highly beneficial. This would be essential for making the transition from traditional concrete structures to nano-engineered cementitious composite. It has already been shown that concrete can be nano-engineered by the incorporation of nano-sized building blocks or objects (e.g. nanoparticles and nanotubes) to control material behaviour and add novel properties (Sobolev and Sanchez, 2010; Sanchez and Sobolev, 2015).

Little has been done on simulating self-healing processes at the nano-scale but some advances have been made in the characterization of the nano-structure of cement-based materials and in computational methods for engineering the structure and the properties of cement-bound materials (Sanchez and Sobolev, 2015).

6. DISCUSSION AND CLOSING REMARKS

One issue that stands out from this review is that many models for SHCMs have been validated using either limited sets of experimental data or no test data at all. In addition, many papers do not review experimentally observed material behaviour in advance of presenting model theory. There are probably a number of reasons for this state of affairs. One could be that there is a paucity of experimental data suitable for properly validating numerical models. Another reason might be that there has been insufficient interaction between relevant numerical and experimental research teams. Whatever the reasons, the authors of this review conclude that there needs to be much closer collaborations between investigators who are developing and testing SCHMs and researchers involved in developing models to predict their behaviour.

The above observation leads on to a discussion about the different ways that mechanical healing is simulated. Amongst the damage-healing models reviewed in Section 2, two different approaches have been taken to the computation of mechanical healing; one considers healing to be a thermodynamic variable whilst the other simulates solidification of the healing agent directly. The evolution of healing in the former approach is treated much like the evolution of damage but with the opposite sign. In the latter approach, damaged material is considered to be a porous medium into which healing agents flow and subsequently harden. For reasons mentioned earlier in this paper, the present authors consider the latter approach to better represent the coupled physico-chemical mechanisms of real healing processes observed in experiments.

A number of authors acknowledge the limitations of their models. Some common restrictions on models for mechanical damage-healing behaviour are that, (i) only one cycle of healing can be simulated, (ii) healing takes place under zero-strain conditions, (iii) damage and healing are never concurrent, and (iv) healing takes place instantaneously. Whilst some of these restrictions are applicable to certain damage-healing scenarios, a comprehensive model would have no such limitations.

One of the particular challenges facing the research community in this area arises from the considerable variability in the micro-structure and material properties of SHCMs. Although recognised by many researchers, the statistical variations of micro-scale components and their associated parameters have only been considered in a few exploratory investigations.

A related issue concerns the huge variability found in published diffusion and permeability coefficients for nominally similar cementitious materials. It seems likely that this issue can only be adequately resolved by a proper consideration of the transport of agents at multiple scales within a statically variable micro-structure.

Models that explicitly represent the micro-structure of SHCMs also show considerable promise in representing the mechanical behaviour of SHCMs. They provide a rational basis for predicting the fracture of micro-capsules and for simulating the formation and healing of micro-cracks.

At the end of this review, the authors consider that the journey towards the development of a set of comprehensive reliable models for self-healing cementitious materials is in its early stages; however, the research undertaken to date shows the potential of models to simulate individual aspects of SH behaviour and represents very considerable progress on numerical methods for simulating a highly complex and statistically variable set of coupled processes.

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