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CIVIL INFRASTRUCTURE

A 3D Coupled Finite Element Model for Self-Healing Quasi-Brittle Materials

This study presents an overview of a 3D coupled finite element model for self-healing quasi-brittle materials. The model was developed alongside a linked experimental programme such that model components were formulated based on observed material behaviour and physical processes. The mechanical model comprises an embedded strong discontinuity element for representing discrete macro-cracks and a linked damage-healing cohesive-zone model. This is coupled to a transport model that simulates the reactive transport of healing agents in both discrete macro-cracks and the surrounding matrix material. For the simulation of the healing reaction that governs crack sealing and mechanical regain, a generalised healing front model is employed. The performance of the model is demonstrated through the consideration of the healing of a cementitious specimen. The results show that the model can accurately reproduce the crack filling predicted by a cement hydration model, and naturally accounts for the effect of healing period and crack width.

Keywords:
Self-healing, numerical modelling, finite element method, concrete, quasi-brittle materials.

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INTRODUCTION

Self-healing materials offer great potential for increased durability, leading to reduced maintenance costs (in terms of both time and money) and increased service life. As a result of this, the development of self-healing quasi-brittle materials such as concrete has been subject to a great deal of interest [1]. Alongside this work, the development of numerical models for simulating the self-healing response has received increasing attention. Whilst initial works focused principally on the mechanical behaviour [2-4], more recent developments have included coupled models that simulate the physical processes governing the healing response [5,6]. It is noted however, that to date no unified model framework for self-healing materials, nor a complete experimental dataset to provide the necessary properties, exists [7].

This study describes a model developed as part of a combined experimental-numerical programme of work. The aim of the work was to develop model components based on an understanding of the physical processes, and to obtain a complete dataset for a particular self-healing system. The experimental work is reported in [8,9], whilst the model components are reported in [10-13]. The work initially focused on a self-healing concrete system with embedded vascular networks and a cyanoacrylate healing agent, though has since been extended to alternative healing systems and agents [13].

This study presents an overview of the model and its extension to healing due to further hydration where multiple healing phases are precipitated within the crack. Model predictions are compared to the results of a cement hydration model (CemPP, a version of CEMHYD3D [14,15]), before an illustrative example concerning a direct tension test, with varying healing crack width and healing periods, is presented.

THEORETICAL BASIS

Model Overview
This study presents an overview a 3D coupled chemo-mechanical finite element model developed to simulate the physical processes governing the self-healing behaviour of quasi-brittle materials such as concrete. The various components of the model include:

- An embedded strong discontinuity element for representing discrete macro-cracks [10],
- A cohesive zone damage-healing model that allows for simultaneous and an arbitrary number of cycles of damage and healing [12],
- An unfitted finite element for representing the healing agent spread in 2D discrete cracks [13],
- A healing agent transport model for flow through the discrete cracks, the surrounding continuum matrix material, and, if present, embedded vascular networks [11,13,16],
- A healing front model for simulating the build-up of healed material, emanating from the crack faces [11,12].

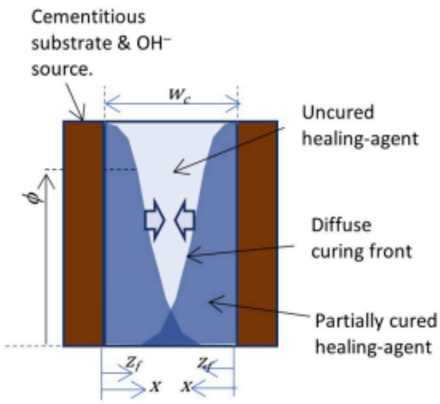

Fig. 1. Conceptual diagram of healing front model that governs crack sealing and mechanical regain (reproduced from [12] with permission)

A conceptual diagram of the healing front model component (that is a key focus of the present work), can be seen in Figure 1.

In the present work, the example problem considered is under saturated conditions and healing and damage occur independently. As such, for brevity, the presentation is focused on the cohesive zone model and healing front model, which herein is extended to the case of multiple healing phases. For further details on the other model components, the interested reader is referred to the papers cited above.

Cohesive Zone Model
The cohesive zone model relates the crack-plane traction vector ($\boldsymbol{\tau_c}$) to the relative displacement vector ($\mathbf{u}$) as follows:

$$\boldsymbol{\tau_c} = (1-\omega)\cdot\mathbf{K}:\mathbf{u} + h\cdot\mathbf{K}:(\mathbf{u}-\mathbf{u}_h) \tag{1}$$

where $\omega \in [0,1]$ is the damage variable, $\mathbf{K}$ is the elastic stiffness, h is the degree of healing and $\mathbf{u}_h$ is the relative displacement at the time of healing. Damage evolution is governed by an exponential softening function [12]:

$$\omega = 1 - \frac{u_t}{\delta} e^{-c\frac{\delta-u_t}{u_m-u_t}} \tag{2}$$

in which $u_t = f_t/K$, where f_t is the tensile strength of the material, $c = 5$ is a softening constant, u_m is the relative displacement at the end of the softening curve and δ is the damage evolution parameter that depends on the maximum value of the inelastic relative displacements.

Mechanical healing is observed once healed material bridges the crack, and -in the absence of re-damage- is given by the total relative area of healed material (φ_{tot}) at the centre of the crack [12]:

$$h(w,t) = \varphi_{tot}(\frac{w}{2}, t) \tag{3}$$

Healing with Multiple Phases

The healing reaction concerns the precipitation of healed material in the crack, emanating from the crack faces. This process can be simulated as the propagation of a diffuse reaction front, and can be described by the following, derived from an analytical solution of the advection-diffusion equation [11]:

$$\varphi_{ph}(x,t) = \frac{\varphi_{ph}^{max}}{2}\left(1 - tanh\left(\left(\frac{2}{\sqrt{\pi}}\right)\left(\frac{x - z(t) - z_{c2}}{z_{c2} + \sqrt{\frac{z(t)}{z_{c1}}}}\right)\right)\right) \tag{4}$$

It is noted that in the present work, we have employed Equation (4) to directly describe the propagation (or build-up) of a diffuse front of healed material, as opposed to considering an advection-diffusion-reaction system. This approach is equivalent to an advection-diffusion-reaction system in which the reaction is sufficiently fast relative to the rates of transport. In this case, the profile of healed material (reaction products) is directly proportional to the concentrations of the reactants. The concentration of the reactants is governed by an advection-diffusion equation with a retardation factor and therefore, the profile of healed material can be described by an advection-diffusion equation.

An illustration of the behaviour of Equation (4) (and Equation (6)) can be seen in Fig. 2.

In (4), x denotes the position measured from the crack face and $z(t)$ is the position of the reaction front given by [11]:

$$z(t) = z_{c0}\left(1 - e^{-\frac{t}{\tau}}\right) \tag{5}$$

where z_{c0} is the critical reaction front depth and τ is the curing time parameter. Finally, z_{c2} is a wall factor and z_{c1} is a diffusion-like coefficient.

In previous works one phase of healed material was considered and the total profile of the relative area of healed material was given by Equation (4) (where $\varphi_{ph}^{max} = 1$). In the present work however, the example considered features multiple phases of healed material and as such, the total profile of the relative area of healed material becomes a summation given by:

$$\varphi_{tot}(x,t) = \sum_{ph=1}^{nph} \varphi_{ph}(x,t) \tag{6}$$

where φ_{ph} is the relative area of healed material of phase ph and nph is the number of healed phases. In addition, φ_{ph}^{max} is the maximum relative area of healed material for phase ph, and it is noted that the condition $\sum_{ph=1}^{nph} \varphi_{ph}^{max} \leq 1$ must be satisfied.

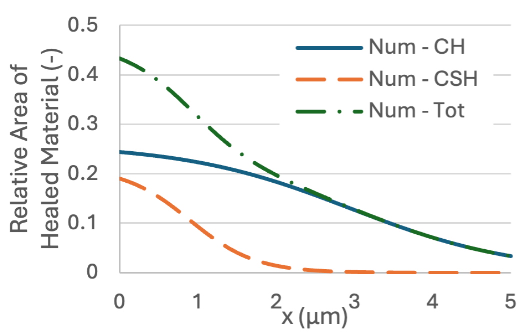

Fig. 2. Illustrative profiles of relative area of healed material as predicted by (4) and (6) (where CH denotes calcium hydroxide, CSH is calcium silicate hydrate and Tot is the total, i.e. CH+CSH).

NUMERICAL IMPLEMENTATION

In the present work the model is implemented in a finite element framework.

For the mechanical behaviour, embedded strong discontinuity elements are employed for the representation of discrete cracks, whilst the nonlinearity is dealt with using a Newton-Raphson procedure [13].

For the transport behaviour, an embedded discrete fracture method is used to describe the coupling between the flow in the porous matrix and the discrete cracks [11], an unfitted finite element method is used to describe the strong discontinuity at the healing agent interface within discrete cracks [13] and the nonlinearity is dealt with using a Picard procedure.

For further details on the numerical implementation, the interested reader is referred to [10-13]. The source code for a 2D version of the model is given in [12].

EXAMPLE PROBLEM

To demonstrate the performance of the model we consider the healing of a cementitious specimen due to further hydration, based on the results presented in [14]. In this example, further hydration leads to precipitation of Calcium hydroxide (CH) and calcium silicate hydrate (CSH) in the crack, with healing observed once the precipitates bridge the crack. In [14], the authors employ the cement hydration model CemPP (CEMHYD3D) to simulate further hydration in a 10μm crack, giving a prediction of the degree of healing as a function of healing time. In the present work, we first employ the healing front model to simulate the healing reaction. Following this, a direct tension test of a double-notched cementitious cube is simulated to illustrate the stress-crack mouth opening displacement (CMOD) response of the model with varying healing periods and CMOD at which healing begins.

The model parameters employed can be seen in Table 1, whilst a schematic of the direct tension test set up is shown in Fig. 3. In [14], the authors found that the degree of mechanical healing was approximately double the degree of healing at the centre of the crack. To reflect this, the mechanical parameters of the healed material were set to double that of the cementitious matrix.

Parameter	Value	Parameter	Value
$E\ (GPa)$	30	$z_{c1,CSH}\ (mm)$	100
$E_h\ (GPa)$	60	$\tau_{CSH}\ (days)$	42
$\upsilon, \upsilon_h\ (-)$	0.3	$z_{c0,CH}\ (mm)$	0.03
$f_t\ (MPa)$	1.5	$z_{c1,CH}\ (mm)$	100
$f_{th}\ (MPa)$	3	$\tau_{CH}\ (days)$	1167
$u_m\ (mm)$	0.02	$z_{c2}\ (mm)$	0.0001
$u_{mh}\ (mm)$	0.0075	$\varphi_{CSH}^{max}\ (-)$	0.25
$z_{c0,CSH}\ (mm)$	0.025	$\varphi_{CH}^{max}\ (-)$	0.324

Table 1. Model parameters.

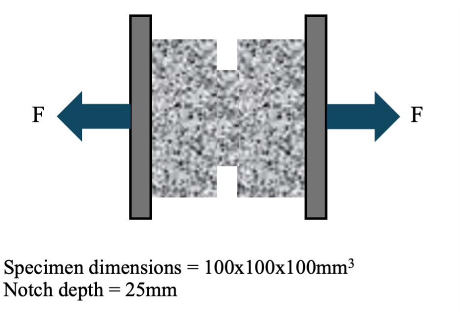

Fig. 3. Schematic of direct tension test.

A comparison between the predictions of the healing front model and the results of [14] can be seen in Fig. 4.

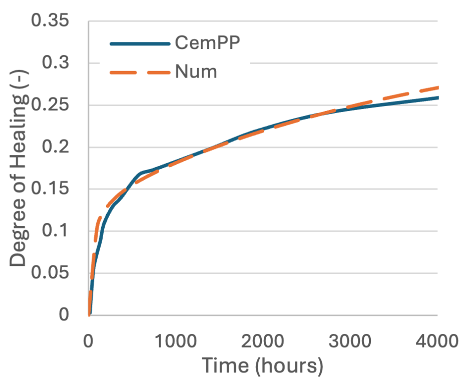

Fig. 4. Degree of healing of 10µm crack as predicted by CemPP [14] and present model.

The results of the direct tension test can be seen in Fig. 5.

DISCUSSION

The examples presented show that the multi-phase healing front model can accurately reproduce the results of the cement hydration model, CemPP (see Fig. 4). In addition, the direct tension test demonstrates that the model can account for both the effects of varying healing period and CMOD at the time of healing (see Fig. 5).

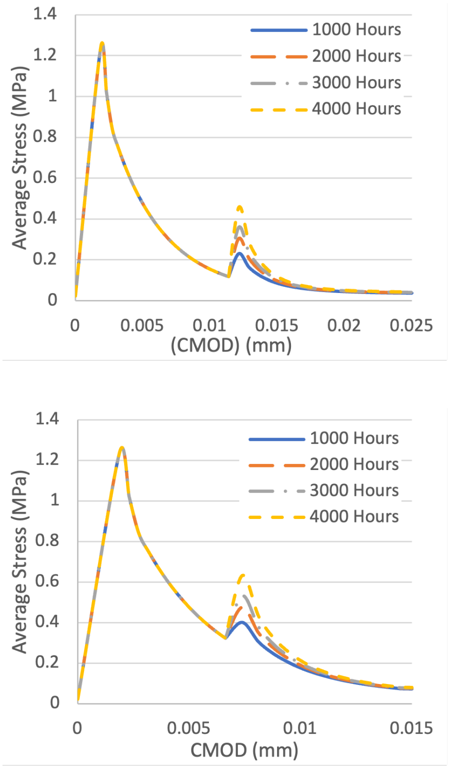

Fig. 5. Predicted Stress-CMOD response different healing periods and at CMODs of a) 0.011mm and b) 0.007mm respectively.

CONCLUSIONS

This study has provided an overview of a couple finite element model, developed as part of a combined experimental-numerical programme, for simulating self-healing quasi-brittle materials. The model features various components for simulating each of the physical processes that govern the healing response. The healing front model for simulating the build-up of healed material in discrete cracks has been extended to the case of multiple healing phases. The performance of the model has been demonstrated through the consideration of an example problem concerning the healing due to further hydration of a cementitious specimen, and its mechanical response in a direct tension test. The results of the example problem show that the extended healing front model can accurately reproduce the predictions of a cement hydration model, and that the coupled model naturally captures the effects of both the healing period and crack opening at the onset of healing.

Future work will investigate the extension of the model to further healing systems and agents.

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Conflicts of interest
The authors declare no conflict of interest.

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