# MICROMECHANICAL SOLUTION FOR SIMULATING AUTOGENOUS HEALING IN CEMENTITIOUS MATERIALS

## (ACME 2016)

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#### ABSTRACT

Self-healing cementitious materials could greatly improve the durability properties of concrete structures relative to those constructed with conventional cementitious composites. However, there is a need to understand better the healing processes, to predict accurately experimental behaviour and to determine the impact on mechanical properties. Micromechanical modelling, with a two-phase Eshelby inclusion solution, is chosen as a suitable framework within which to explore such a response in cementitious materials. A constitutive material model is described, consideration is given to a self-healing model framework and how the mechanical strength recovery of a micro-cracked material can be simulated with a simplified volumetric micromechanical model.

Keywords: micromechanics; micro-cracking; healing; cementitious

#### 1. Introduction

Micromechanics is a technique are used to describe engineering material properties based on basic continuum mechanic concepts; conservation of mass and balance of momentum and energy. Micromechanical models allow the individual material properties, damage and inelastic response to be modelled at the same length scale whilst also linking to the macroscale. This paper simulates a two-phase composite material which has a matrix phase and inclusions. The particular focus is on building a framework for simulating healing in a cracked material.

In recent years much research has been undertaken on the subject of self-healing in cementitious materials [1], [2]. A number of models have been developed for simulating self-healing behaviour [3]–[6]. The majority of the mechanical healing models developed to date are phenomenological in nature and have been applied in finite element codes using the smeared crack concept. However, the present authors favour more mechanistic approach. In cementitious materials, the development of material properties and recovery can be linked to the hydration process, particularly for early age crack healing. Hydration processes and damage have been considered in a coupled model [7] where the evolution of healing was linked to both the degree of hydration and to the value of the damage parameter at time of healing.

A micro-scale model naturally captures the early stages of micro-cracking and the extent of damage in the fracture process zone around a macro-crack by considering the behaviour of the composite components. A model which can represent micro-cracks is ideally suited for including self-healing behaviour by healing these explicit cracks.

## 2. Essential components of the micro-mechanical model

A cementitious material with aggregate particles and cement paste is represented using a two phase composite with inclusions ( $\Omega$ ) and a matrix (M) phase. A detailed description of the basic micromechanical model can be found in [8], [9]and [10]. The essential components of the micromechanical model are shown in the following constitutive equation and are taken forward to establish a framework for instructing healing:

$$\overline{\mathbf{\sigma}} = \mathbf{D}_{M\Omega} : (\overline{\mathbf{\varepsilon}} - \mathbf{\varepsilon}_{\mathbf{a}}) \tag{1}$$

 $\overline{\sigma}$  is the average stress and  $\overline{\epsilon}$  is the total strain in the composite.  $\mathbf{D}_{M\Omega}$  is the composite elastic tensor whose properties are computed using the classical Eshelby [11] solution and the Mori-Tanaka homogenization scheme for non-dilute inclusions [12].  $\boldsymbol{\epsilon}_{a}$  is the total additional strain resulting from anisotropic micro-cracking using the approach of Budiansky and O'Connell [13]. A local stress-strain relationship for the micromechanical model is defined in equation (2), in which the added strain is taken to be the equivalent of a micro-cracked band in the material.

$$\mathbf{s}_{L} = (1 - \omega) \mathbf{D}_{L} \mathbf{\varepsilon}_{L} \tag{2}$$

 $\mathbf{s}_{L}$  is the equivalent local stress tensor and  $\mathbf{\varepsilon}_{L}$  is the equivalent local strain tensor, both of which are expressed in a reduced vector form that considers only those components that are non-zero.  $\mathbf{D}_{L}$  is a 3x3 matrix containing the non-zero components the local stiffness tensor. The local compliance tensor is defined as  $\mathbf{C}_{L} = \mathbf{D}_{L}^{-1}$ .  $\boldsymbol{\omega}$  is the micro-crack variable for each direction, taking the values between 0 for uncracked and 1 for the fully micro-cracked state. The elastic local strain can be subtracted from the local strain within the micro-crack band ( $\mathbf{\varepsilon}_{L}$ ) to give the additional strain resulting from the crack in one direction.

#### 3. Self-healing model framework

The local constitutive relationship presents itself as a convenient form for including healing. The healing restores the stiffness of a proportion of the damaged component of material. An offset or 'solidification' strain is included to ensure that the healing material solidifies in a stress free state. The healed local stress is given in equation (3).

$$\mathbf{s}_{Lh} = (1 - \omega) \mathbf{D}_L \boldsymbol{\varepsilon}_{Lh} + (1 - \omega_h) h \omega_{th} \mathbf{D}_{Lh} (\boldsymbol{\varepsilon}_{Lh} - \boldsymbol{\varepsilon}_s)$$
(3)

The healing proportion is defined by the parameter *h*, which takes the values between 0 for no healing and 1 for fully healed. A subscript *h* is added to the terms to show the healing equivalent terms.  $\mathbf{s}_{Lh}$ is the equivalent local stress tensor after healing,  $\mathbf{\varepsilon}_{Lh}$  is the local equivalent strain tensor after healing and  $\omega_{th}$  is the micro-cracking parameter at the time of healing.  $\mathbf{D}_{Lh}$  is the local stiffness of the healed material and  $\mathbf{\varepsilon}_s$  is the 'solidification' strain. Since this newly healed material can also undergo microcracking, a term is also included to simulate this further micro-cracking, where  $\omega_h$  is the healed micro-cracking variable.

#### 4. Self-healing model volumetric example

A volumetric isotropic model is used here to give an insight into how the model responds to a strain path. The single phase volumetric constitutive relationship is shown in equation (4), which has the same basic form as that given in equation (3).

$$\sigma = (1 - \omega) K_M \varepsilon + (1 - \omega_h) h \omega_{th} K_{Mh} (\varepsilon - \varepsilon_s)$$
<sup>(4)</sup>

 $K_M$  and  $K_{Mh}$  are the bulk modulus of the material before and after healing. All other terms remain as previously defined. The material properties used are shown in Table 1. The original and healed micro-crack initiation and evolution criteria are based on the form adopted by Mihai & Jefferson [8] and are

based on;  $\varepsilon_{tv}$  which is the volumetric strain at first uniaxial micro-cracking and  $\varepsilon_{0v}$  which is the volumetric uniaxial local strain in the effectively fully micro-cracked state. This model is subjected to a volumetric strain increment where both micro-cracking parameters are calculated directly.

$\frac{K_{M}}{(N / mm^{2})}$	$\frac{K_{Mh}}{(N / mm^2)}$	$\mathcal{E}_{tv}$	$\mathcal{E}_{tvh}$	$\mathcal{E}_{0v}$	$\mathcal{E}_{0v}$	h
11429	5714	$4.17 \times 10^{-5}$	$8.33 \times 10^{-5}$	$6.67 \times 10^{-3}$	$6.67 \times 10^{-5}$	0.5

Table 1: Material properties for volumetric model response

The volumetric strain is incremented until the original material reaches a point on the loaddisplacement (stress-strain) softening curve equal to half the peak stress, after which the strain is returned to zero. This strain response is shown in Figure 1. The healing here is assumed to take place when the sample is unloaded which occurs when there is zero stress and zero strain. For the time strain plot shown in Figure 1, this unloading point occurs at a pseudo-time t = 1000(s). At this point the  $\varepsilon_s$  is zero and the  $\omega_{th}$  is fixed. The new material incorporating the healing is then subjected to further strain increments up to and beyond the initial peak strain, until the strain is four times the original unloading strain. Figure 2 shows the stress strain response of the volumetric healed model. The first loading phase, up to t = 1000(s), can be seen where the stress returns along a linear line to zero. The second loading phase shows a bi-linear line returning to the softening curve (in stress-time space) of the healed material. This increase in stress directly relates to the healed material. The first steep gradient is due to the elastic response of the healed material and the second flatter gradient is the sum of stresses in both materials. The peak stress after healing is reached at the same strain at which the model was first unloaded, this being t = 1500(s).



Figure 1: a) Volumetric strain driver b) Typical volumetric stress strain healing response

#### 5. Conclusions

A two phase composite micro-mechanical constitutive model, that includes anisotropic microcracking, provides an excellent basis for the development of a model for cementitious materials that includes self-healing behaviour. The relative simplicity of this micromechanical healing model combined with the fact that it requires a small number of physically meaningful parameters shows that it is suitable for simulating a wide range of two-phase cementitious materials. The volumetric example shown is useful to illustrate the mechanisms that occur during the micro-cracking and healing processes.

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