The simulation of time dependent behaviour of cement bound materials with a micro-mechanical model

Numerical Modeling Strategies for Sustainable Concrete Structures
Aix-en-Provence, France
May 29-June 1, 2012

R. Davies, A.D. Jefferson

Cardiff School of Engineering, Cardiff University, Cardiff, Wales, UK

1. Abstract

An approach is described for simulating the behaviour of concrete, and other cementitious composites materials, using micro mechanics. The basic mechanical material model is that presented by Mihai and Jefferson[1] which employs micromechanical solutions of a two-phase composite comprising a matrix phase, spherical inclusions, circular microcracks distributed in the matrix and potentially combining these with a rough crack contact component. The primary focus of the paper is on the enhancement of the model to allow for the future inclusion of time dependent behaviour. This is accomplished by the addition of inelastic strains in the matrix phase. These inelastic strains can be included at the fundamental micromechanical level of the homogenisation process by being included in the compatibility equations and embedded mechanistically into the constitutive equations.

2. Introduction

The theory of Micromechanics is used to describe engineering material properties, which is based on basic continuum mechanics concepts; conservation of mass and balance of momentum and energy. Micromechanical approximation techniques are particularly suited to modelling cementitious materials due to their inhomogeneous nature[2]. The techniques used include damage or plasticity theories, phenomenological or mechanistic approaches and differing length scales of the material.

The dominant time dependent mechanisms occurring in concrete are shrinkage and creep. These mechanisms all produce inelastic strains within the material. The creep and shrinkage which occur in concrete have been proven to only occur within the matrix phase[3]. The shrinkage strains result in isotropic stresses, which result directly from moisture loss. Creep is considered to behave in a visco-elastic manner. Therefore concrete can be represented by an inelastic composite consisting of elastic aggregate inclusions and an inelastic mortar matrix.

There are several micromechanical models which deal with these inelastic strains in cementitious materials. Benboudjema et al[4] present a two-scale micromechanical constitutive model, which has two damage variables, considers shrinkage and creep strains as inelastic strains in a one phase material. The elastic stiffness tensor remains the same throughout.

Scheiner and Hellmich[5] and Pichler et al[6] use a homogenisation-based multi-scale concepts. Pichler et al[6] arrives at shrinkage strains in the matrix material by up-scaling effective elastic properties from the cement paste scale and similarly from the calcium-silicate-hydrate level. The classical Eshelby solution is used with the Mori-Tanaka scheme to estimate the homogenized bulk and shear relaxation moduli of the different length scale models. The self-consistent homogenisation approach is used where the length scale relates to that of the crystalline structure and Laplace-Carson transformations are used in the integration of the visco-elastic creep expressions.

The present paper explores different methods of including the inelastic terms into a composite material. This paper has been developed considering a 3D micromechanical model with the ability to apply anisotropic loading. Essential ideas described by Jefferson and Bennett[7,8] are employed whilst adopting the more mechanistic approach of Jefferson and Mihai[1].

The particular focus of this paper is to explore the introduction of these inelastic strains into the matrix component of the two-phase model. A brief description of the basic model and different methods of applying shrinkage and creep in the matrix will be presented first. A standard solution is given for the proposed approach, before considering specific application to shrinkage and creep.

3. Basic modelling approach

The two-phase composite model by Jefferson and Bennett[8] and further developed into a mechanistic model by Jefferson and Mihai[1] will form the basis of the micromechanical model. These models employ micromechanical solutions of a two-phase composite comprising a matrix phase, spherical inclusions, and circular microcracks distributed in the matrix.

The basic elastic solution and associated assumptions are briefly discussed, before moving on to the inelastic composites. The work discussed in this paper is for a 3D micromechanical model and the direct tensor notation applies. A two-phase composite model of concrete has been adopted, where the matrix material (M) represents the mortar and spherical inclusions (Ω) represent coarse aggregate particle. The two-phase homogenisation of the composite has been carried out using the classical Eshelby (1957) solution and applying the Mori-Tanaka homogenisation for non-dilute inclusions. The damage is accounted for with the addition of strain due to penny shaped microcracks.

3.1. Elastic two-phase composite

Upon homogenisation the average stress and average strain are given by equations (1) and (2) in which the sum of the volume fractions (f_Ω and f_M) equals unity.

$$\bar{\sigma} = f_\Omega \cdot \sigma_\Omega + f_M \cdot \sigma_M \tag{1}$$

$$\bar{\varepsilon} = f_\Omega \cdot \varepsilon_\Omega + f_M \cdot \varepsilon_M \tag{2}$$

The classical Eshelby solution essentially replaces an inclusion with an equivalent inclusion made from a matrix material. Application of the Mori-Tanaka homogenisation scheme for non-dilute inclusions results in the average stress-strain relationship shown in equation (3) below.

$$\bar{\sigma} = D_{M\Omega} : \bar{\varepsilon} \tag{3}$$

$$\text{where} \quad D_{M\Omega} = \left(f_\Omega \cdot D_\Omega : T_\Omega + f_M \cdot D_M\right)\cdot\left(f_\Omega \cdot T_\Omega + f_M\right)^{-1} \tag{4}$$

$$\text{and} \quad T_\Omega = I^{4s} + S_\Omega : A_\Omega \tag{5}$$

$$\text{and} \quad A_\Omega = \left[(D_\Omega - D_M) : S_\Omega + D_M\right]^{-1} : (D_\Omega - D_M) \tag{6}$$

$$\text{and} \quad f_M + f_\Omega = 1 \tag{7}$$

D_M, D_Ω and $D_{M\Omega}$ are the elastic stiffness constants in the matrix, inclusion and composite respectively. T_Ω and A_Ω are constants which allow the expressions to be simplified. The interior point fourth order Eshelby tensor is represented by S_Ω, where standard solutions are available for the spherical inclusions. The S_Ω is used to relate the eigenstrain to the constrained strain as shown by equation (8).

$$\varepsilon_c = S_\Omega : \varepsilon_\tau \tag{8}$$

3.2. Additional Strain due to penny shaped microcracks

A dilute distribution of penny shaped micro-cracks was introduced following the classical approach of Budiansky and O'Connell[9]. The damage resulting from these microcracks adds a cracking strain (ε_a) to the total composite strain equation (9). The added cracking strain is included in the standard constitutive equation (10), where the total strain is the sum of the elastic total strain and the added cracking strain.

$$\bar{\varepsilon} = f_M \cdot \varepsilon_M + f_\Omega \cdot \varepsilon_\Omega + \varepsilon_a \tag{9}$$

$$\bar{\sigma} = D_{M\Omega} : \bar{\varepsilon}_e = D_{M\Omega} : (\bar{\varepsilon} - \varepsilon_a) \tag{10}$$

The steps employed in determining these added micro-cracks are comprehensively presented by Jefferson and Bennett [8]and Jefferson and Mihai[1]. Essentially, the Budiansky and O'Connell crack density parameter is replaced by a directional damage parameter (ω). Unit local coordinate vectors are used with an elastic compliance tensor (C_L) to produce a local added micro-cracking strain component (ε_α). The local cracking strain component (11), in terms of directional damage and local stress vector (s) is derived from the sum of the local strain and local elastic strain.

$$\varepsilon_\alpha = \left(\frac{\omega}{1-\omega}\right) C_L : s \tag{11}$$

The total added micro-cracking strain (ε_α) is achieved by the standard solution of integrating around a hemisphere. This is implemented numerically by the 29-point McLauren Rule[10]. The constitutive equation including the total micro-cracking component is represented by the secant constitutive equation (12). The N_ε and N are the stress and strain direction transformations as employed previously by Jefferson[11].

$$\bar{\sigma} = D_{\sec} : \bar{\varepsilon} \tag{12}$$

where

$$D_{\sec} = \left[1 - \frac{1}{2\pi} \int_{2\pi} \int_{\frac{\pi}{2}} N_\varepsilon : C_L : N \cdot \frac{\omega(\theta,\psi)}{1-\omega(\theta,\psi)} \sin(\psi) d\psi d\theta \right]^{-1} \cdot D_{M\Omega} \tag{13}$$

3.3. Basic model extensions

A number of variations have been considered on the above basic model. These variations include the rough contact model for stress recovery[7] and including the later work of Eshelby (1959), which is the exterior point Eshelby for stress outside and inclusion[1]. The crack initiation criterion and evolution function have also been examined in detail with respect to the inclusion of inelastic strain, in particular where the initial microcracks occur in the matrix material.

4. Different methods of applying shrinkage and creep into the matrix only

Firstly, techniques for including inelastic strains in inclusions are discussed by Nemat-Nasser and Hori [9], Mura [12] and Weng [13], where all authors achieve a similar solution using a relatively straight forward approach. The inelastic deformation takes place within the inclusion and is present either side of the consistency equation using the equivalent inclusion method. The constrained strain associated with this approach is shown in equation (14) and it is noted that the inclusion's inelastic strain impacts on the matrix through the constrained strain equation only.

$$\varepsilon_c = S_\Omega : (\varepsilon_\tau + \varepsilon_i) \tag{14}$$

Weng [13] presents a range of methods to represent plasticity in composites. Two of these specifically address the elastic inclusion and plastic matrix problem: the secant moduli tensor approach and the elastic constraint approach.

The secant moduli tensor approach, takes the reducing restraining effect of the matrix on the inclusion into account by the reducing stiffness of the secant moduli by a plastic strain. The consistency equation is setup in a similar manner to the elastic composite but the matrix stiffness moduli is replaced by the secant moduli. These secant moduli can be applied to a plastic strain which in turn can is related to the stress. The constrained strain associated with the secant method is shown in equation (15). The inelastic shrinkage strain cannot be related directly to stress and as such this secant moduli tensor approach was discounted for the present work. However, the approach has some attractions when modelling creep and has been applied to a logarithmic creep model[14].

$$\varepsilon_c = S_{secant} : (\varepsilon_\tau) \tag{15}$$

In the elastic constraint approach, the plastic strain in the matrix is transferred to the inclusion using compatible deformations and these deformations appear in the inclusion consistency equation as a positive strain. This plastic strain also appears in the constrained strain as a negative plastic strain. This approach is in contrast to the standard inelastic inclusion composite derivations, where here the inelastic matrix strain impacts on the inclusion through the constrained strain and equivalent deformation. The elastic constraint method provides a stiffer response than the secant method as expected. Ward[15] developed the work of Weng by using a secant tangent stiffness approach with an incremental elasto-plastic flow rule.

5. Standard solution for a two-phase composite with inelastic strain in the matrix only

The inelastic strain has only been incorporated into the matrix phase of the composite material. The process of deriving the constitutive model is shown, focusing on the inelastic assumptions. The additional strain due to microcracking, and how this will be implemented with inelastic strains in the matrix, is discussed.

5.1. Individual phase equations

Each phase within the composite material can be addressed in their individual constitutive equations (16) and (17). The total elastic strain in the matrix is formulated from the farfield strain (ε_o), constrained strain (ε_c) and the inelastic strain (ε_i). Therefore, the stress in the matrix contains the inelastic strain. By applying Eshelby's equivalent inclusion method to the inclusion constitutive equation, the transformation strain (ε_τ) which takes account of the different materials is introduced. This format is often referred to as the constancy equation (17).

$$\sigma_M = D_M : \varepsilon_M = D_M : (\varepsilon_o + \varepsilon_c - \varepsilon_i) \tag{16}$$

$$\sigma_\Omega = D_\Omega : \varepsilon_\Omega = D_\Omega : (\varepsilon_o + \varepsilon_c) = D_M : (\varepsilon_o + \varepsilon_c - \varepsilon_\tau) \tag{17}$$

Combining the effect of the inelastic strain and the transformation strain, the constrained strain is defined in equation (18). This relationship was developed from first principles by considering inelastic strain in the inclusion, then a homogeneous composite material before introducing the inelastic strain into the matrix. In comparison with the standard model (3.1), the additional term in equation (18) is the inelastic strain.

$$\varepsilon_c = S_\Omega : (\varepsilon_\tau - \varepsilon_i) \tag{18}$$

Substituting in equation (18) into equation (17) and rearranging to get the transformation eigenstrain in terms of the farfield strain and inelastic strain yields the following relationship.

$$\varepsilon_\tau = A_\Omega : (\varepsilon_o - S_\Omega : \varepsilon_i) \tag{19}$$

$$\text{where } A_\Omega = \left[(D_\Omega - D_M) : S_\Omega + D_M\right]^{-1} : (D_\Omega - D_M) \tag{20}$$

Note that the A_Ω term remains the same as for the standard elastic solutions. The relationship for the stress in the inclusions can then be expressed by substituting this eigenstrain relationship into the relevant stress equations eliminating the transformation strain from the standard equation.

5.2. Individual phase equations – applying Mori-Tanaka averaging

In considering the individual phase equations the Mori-Tanaka method[9] uses an argument whereby the inclusions are not dilute and therefore the 'disturbance' strain may be based on the average matrix stress (or strain) rather than the farfield stress (or strain). Therefore, for the matrix phase, the far field strain (ε_o) and disturbed strain (ε_c) in equation (16) can be replaced by the strain in the matrix (ε_M). Applying the Mori-Tanaka theory to equation (16) leads to the following relationship for the stress in the matrix material (21).

$$\sigma_M = D_M : (\varepsilon_M - \varepsilon_i) \tag{21}$$

The stress in the matrix can also be compared to the standard Hooke's Law for the matrix phase. It is noted that the displacement in the matrix phase is the sum of the matrix elastic component and the matrix inelastic component.

$$\varepsilon_{Mel} = \varepsilon_M - \varepsilon_i \quad \text{or} \quad \varepsilon_M = \varepsilon_{Mel} + \varepsilon_i \tag{22}$$

For the inclusion phase, only the far field strain (ε_o) is replaced by the strain in the matrix (ε_M). The disturbed strain (ε_c) remains in place. Applying the Mori-Tanaka theory and substituting equations

(18) and (19) into both sides of the consistency equation, the following relationships for the stress in the inclusions is achieved (23).

$$\sigma_\Omega = D_\Omega : T_\Omega : (\varepsilon_M - S_\Omega : \varepsilon_i) \qquad \text{where } T_\Omega = I^{2s} + S_\Omega : A_\Omega \tag{23}$$

5.3. Overall composite equations

The constitutive equation can be constructed by eliminating the individual component stresses or strains from the homogenisation equations. Substituting the inclusion strain into the total strain equation (2) and isolating the matrix strain yields a relationship (24), which can be further substituted into the stress balance equation.

$$\varepsilon_M = \left(f_\Omega \cdot T_\Omega + f_M\right)^{-1} : (\bar{\varepsilon}_T + f_\Omega \cdot T_\Omega \cdot S_\Omega : \varepsilon_i) \tag{24}$$

Substituting in (21), (23) and (24) into the stress balance equation (1), the following constitutive equation for an elastic composite material is produced.

$$\bar{\sigma} = D_{M\Omega} : (\bar{\varepsilon} - \varepsilon_{INEQ}) \tag{25}$$

where $$D_{M\Omega} = \left(f_\Omega \cdot D_\Omega : T_\Omega + f_M \cdot D_M\right) \cdot \left(f_\Omega \cdot T_\Omega + f_M\right)^{-1} \tag{26}$$ and

$$\varepsilon_{INEQ} = D_{M\Omega}^{-1} \cdot \left(-D_{M\Omega} \cdot f_\Omega \cdot T_\Omega : S_\Omega + f_\Omega \cdot D_\Omega \cdot T_\Omega : S_\Omega + f_M \cdot D_M\right) : \varepsilon_i \tag{27}$$

The rigorous addition of the inelastic strain in the matrix material, worked through to the average constitutive equation, leads to a complex solution as shown by equation (27). It can be seen that the constitutive equation is impacted upon by the inelastic strain in the matrix relative to the volume fractions of the material.

5.4. Additional Strain due to penny shaped microcracks

The additional strain due to penny shaped microcracks can be employed in a similar manner to (3.2) where the inelastic strain is included in the total elastic strain component of equation (25).

$$\bar{\sigma} = D_{M\Omega} : (\bar{\varepsilon} - \varepsilon_{INEQ} - \varepsilon_a) \tag{28}$$

The constitutive equation (28) can be re-arranged into a secant stiffness matrix as follows, where D_{sec} is the same as equation (13).

$$\bar{\sigma} = D_{\sec} : (\bar{\varepsilon} - \varepsilon_{INEQ}) \tag{29}$$

6. Shrinkage in isolation

The inelastic shrinkage strain for this model has been based on an exponential drying curve derived from experimental data from a concrete with water/cement ratio of 0.55[16] and the volumetric shrinkage rate is assumed to be linearly related to the moisture change rate.

Typical material parameters used to illustrate the performance of the micromechanical model are shown in Table 1.

Table 1: Material parameters

f_M	E_M (N/mm^2)	ν_M	f_Ω	E_Ω (N/mm^2)	ν_Ω	μ_s	ε_o	c (N/mm^2)	f_t (N/mm^2)
0.6	32 000	0.1	0.4	49 000	0.28	1	0.003	2.5	1

A free shrinkage the model was simulated and individual material phases are presented in Figures 1a/b. An assumption was made in that no microcracking would occur to allow the model to be tested.

Figure 1a/b shows the variation of the driver shrinkage strain along with the strains in the inclusion, matrix and the average composite strain, as well as the associated stresses. As expected, without cracking, the ratio of the components remains constant. The average strain of the composite is in proportion to the volume factors between the matrix and inclusion. The positive matrix elastic strain represents the tensile stress which will be subjected to microcracking. Figure 1b shows the stress in the inclusion being higher than in the matrix. The stress in the composite on the whole remains zero.

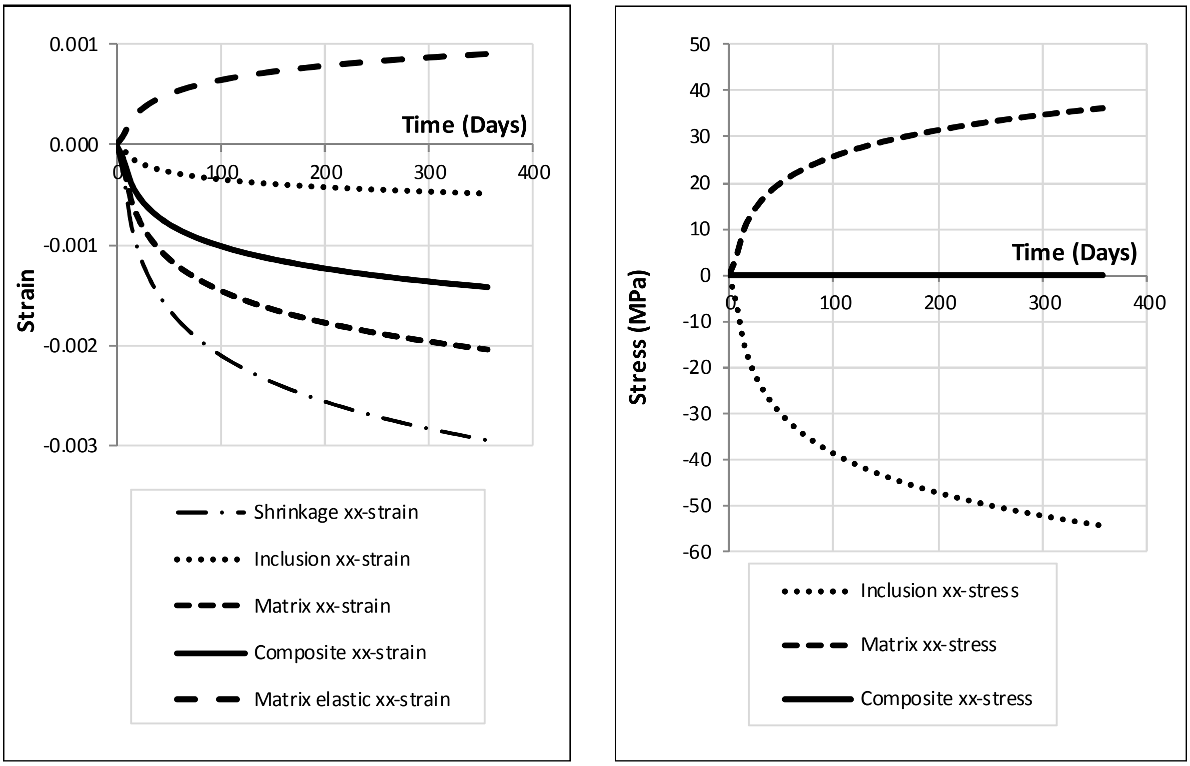

Figure 1a/b: Strain and stress in the composite developing with time in the x-x direction

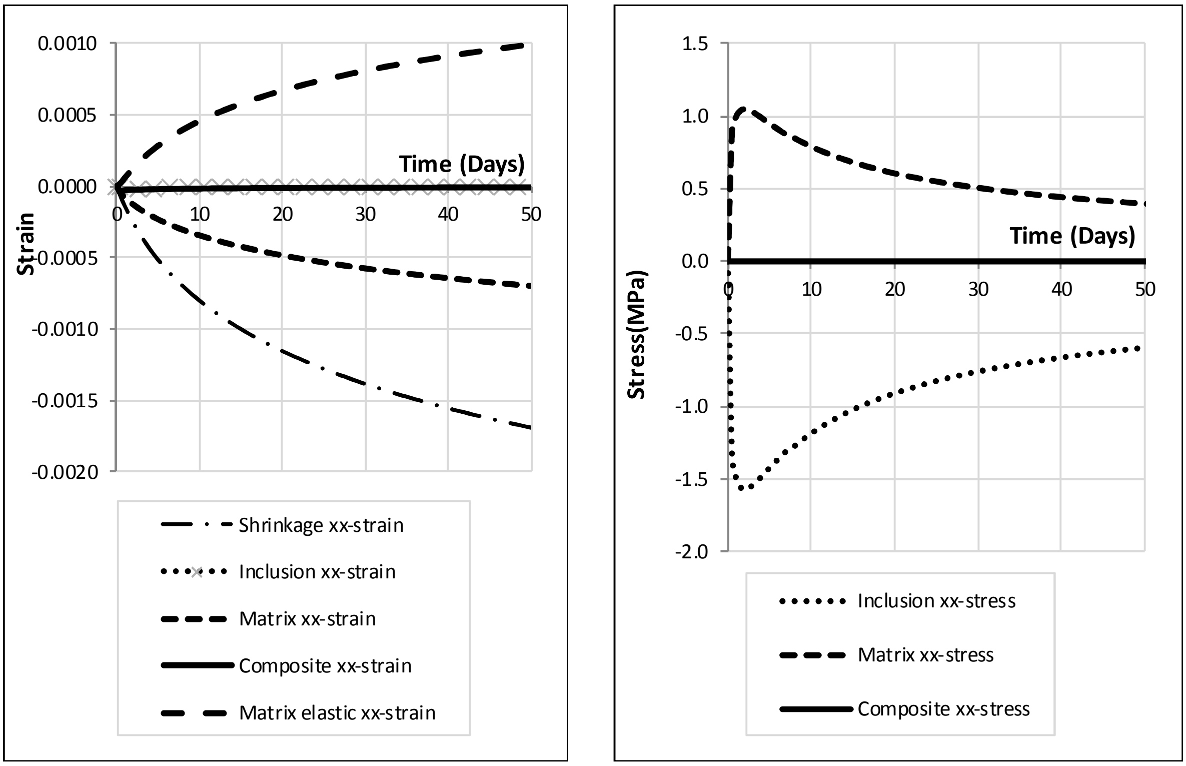

Figure 2a/b: Strain and stress in the composite with microcracking developing with time in the x-x direction

Figure 2a/b shows the effect of the driver shrinkage strain with microcracking on the strains in the inclusion, matrix and the average composite strain, as well as the associated stresses. The stains in the inclusion and composite are very small with the inclusion of microcracking. Figure 2b shows the effect of microcracking in the composite in response to shrinkage in the matrix where the characteristic strain softening curve is found in the matrix and inclusion stresses and the total stress remains at zero. These figures show that material reaches maximum stress after a few days of shrinkage. It is recognised that there will be a dramatic reduction in stress when considering microcracking and creep.

These illustrations show how the shrinkage equations impact on an idealised material. It is recognised that the effect of early age properties or creep are not included. However, these simulations do illustrate the basic predictions of the equations where the inelastic strains are included in the matrix material.

7. Creep

The authors have developed a new micro-mechanical creep model which uses the ideas from the solidification theory[17] -and which accounts for the recent observations on the fundamental nature of creep by Jennings & Bullard[18] and Vandamme & Ulm et al[19] -to develop a model based on developing pairs of Maxwell rheological units. The resulting inelastic creep strains are treated in essentially the same manner as the shrinkage strains described above. This work is to be the subject of a future publication.

8. Concluding remarks

The micromechanical model is described where inelastic strains are introduced into the matrix component of a two-phase cementitious composite model. A new way of introducing inelastic strains into the matrix is described from first principles and this has been tested using a shrinkage strain.

The performance of the equations presented in this paper are illustrative. These show that the equations predict the expected shrinkage behaviour of a two-phase composite when the shrinkage is restricted to the matrix alone with and without microcracking.

References

1. Mihai IC, Jefferson AD. A material model for cementitious composite materials with an exterior point Eshelby microcrack initiation criterion. *International Journal of Solids and Structures*. 2011;48:3312-3325.

2. Bohm HJ. A short introduction to basic aspects of continuum micromechanics. *CDL-FMD Report*. 1998;3.

3. Acker P, others. Micromechanical analysis of creep and shrinkage mechanisms. In: *Creep, shrinkage and durability mechanics of concrete and other quasi-brittle materials. Proceedings of the sixth international conference concreep6.[Links]*.; 2001.

4. Benboudjema F, Meftah F, Sellier A, Torrenti JM, Heinfling G. On the prediction of delayed strains for concrete subjected to drying and loading simultaneously. *Proc. CONCREEP: Creep, shrinkage and durability mechanics of concrete and other quasi-brittle materials*. 2001;6:245–250.

5. Scheiner S, Hellmich C, others. Continuum microviscoelasticity model for aging basic creep of early-age concrete. *Journal of Engineering Mechanics*. 2009;135:307.

6. Pichler C, Lackner R, Mang HA. A multiscale micromechanics model for the autogenous-shrinkage deformation of early-age cement-based materials. *Engineering fracture mechanics*. 2007;74(1-2):34–58.

7. Jefferson AD, Bennett T. Micro-mechanical damage and rough crack closure in cementitious composite materials. *Int. J. Numer. Anal. Meth. Geomech.* 2007;31(2):133-146.

8. Jefferson AD, Bennett T. A model for cementitious composite materials based on micro-mechanical solutions and damage-contact theory. *Computers & Structures*. 2009.

9. Nemat-Nasser S, Hori M. *Micromechanics : overall properties of heterogeneous materials*. Amsterdam ;;New York: North-Holland; 1993.

10. Stroud AH. *Approximate Calculation of Multiple Integrals*. Prentice Hall; 1972.

11. Jefferson AD. Craft—a plastic-damage-contact model for concrete.I. Model theory and thermodynamic considerations. *INTERNATIONAL JOURNAL OF SOLIDS AND STRUCTURES*. 2003;40:5973–5999.

12. Mura T. *Micromechanics of defects in solids*. 2nd ed. Dordrecht Netherlands ;;Boston ;Hingham MA USA: M. Nijhoff ;;Distributors for the U.S. and Canada Kluwer Academic Publishers; 1987.

13. Weng GJ. Theoretical principles for the determination of two kinds of composite plasticity- Inclusions plastic vs. matrix plastic. *Mechanics of composite materials- 1988*. 1988:193–208.

14. Pichler C, Lackner R. A multiscale creep model as basis for simulation of earlyage concrete behavior. *Computers and Concrete*. 2008;5(4):295–328.

15. Ward WF. Theoretical Investigation Into the Inelastic Behavior of Metal-Matrix Composites. Final Report for June 1988-June 1990. Master's Thesis. 1990.

16. Cement and Concrete Association Australia. Concrete Data - Drying Shrinkage of Cement and Concrete. 2002.

17. Bazant ZP, Cusatis G, Cedolin L. Temperature effect on concrete creep modeled by microprestress-solidification theory. *Journal of Engineering Mechanics-Proceedings of the ASCE*. 2004;130(6):691–699.

18. Jennings HM, Bullard JW. From electrons to infrastructure: Engineering concrete from the bottom up. *Cement and Concrete Research*. 2011.

19. Vandamme M, Ulm FJ, Fonollosa P. Nanogranular packing of CSH at substochiometric conditions. *Cement and Concrete Research*. 2010;40(1):14–26.