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SMOOTHED CONSTITUTIVE MODEL FOR CONCRETE BASED ON MICROMECHANICAL SOLUTIONS

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Abstract: New developments for simulating microcracking in cementitious composite materials – such as concrete – are presented. A micromechanical constitutive model for concrete is proposed which employs the classic Eshelby inclusion solution and a Mori-Tanaka homogenization scheme to simulate a two-phase composite comprising a matrix phase representing the mortar and spherical inclusions representing the coarse aggregate particles. Furthermore the material contains randomly distributed penny-shaped microcracks. The onset of cracking is addressed in a microcrack initiation criterion, governed by an exterior-point Eshelby solution, in which microcracks are assumed to initiate in the interfacial transition zone between aggregate particles and cement matrix [1]. The adopted solution captures tensile stress concentrations in the proximity of inclusion – matrix interfaces in directions lateral to a compressive loading path. An advantage of the two-phase formulation is that it is able to predict the build-up of tensile stresses within the matrix phase under uniaxial compression stresses thus allowing the model to naturally simulate compressive splitting cracks. The implementation of the microcrack initiation criterion into the constitutive model enables the use of realistic material properties in order to obtain a correct cross-cracking response.

The model combines these solutions with a rough crack contact component which enables it to capture the dilatant behaviour of concrete subject to compression. A novel aspect of the present work deals with the development of a smoothed contact state function in order to remove spurious contact chatter behaviour at a constitutive level. It is shown, based on numerical predictions of uniaxial and biaxial behaviour that the model captures key characteristics of mechanical behaviour of concrete.

1 INTRODUCTION

Considerable research has been carried out since the late 1960's for developing models and techniques to simulate the mechanisms leading to failure of quasi-brittle materials such as concrete. Although the progress achieved during this time is considerable, as yet, no one model has been able to fully capture all facets of the complex mechanical behaviour of concrete.

Concrete modelling at a constitutive level can be classified in two main categories: macroscopic models that follow a phenomenological approach and models based on micromechanical solutions. Phenomenological models generally employ theories based on plasticity and/or damage mechanics in order to simulate the macroscopic behaviour and their formulation often makes use of functions obtained by fitting experimental data (e.g. uniaxial tension and compression curves, strength envelopes). By contrast, micromechanical models aim to relate the microstructure of concrete, and the physical mechanisms that govern its evolution, to the macroscopic behaviour observed in experiments.

The work presented here follows on from the micromechanical constitutive models proposed by Jefferson and Bennett [2,3] - based on Budiansky and O'Connell's [4] solution for an elastic solid containing penny-shaped microcracks and on the Eshelby matrix-inclusion solution- and by Mihai and Jefferson [1] which additionally employed the exterior point Eshelby solution in a microcrack initiation criterion. The model also features a rough crack contact component that accounts for the recovery of stiffness when microcrack surfaces regain contact. The novel aspect in the present work deals with the formulation of a smoothed contact state function to replace the discrete formulation employed in [1-3] in order to remove spurious chatter behaviour.

2 MICROMECHANICAL CONSTITUTIVE MODEL

A full account of the constitutive model is presented in [1] however the main assumptions and key equations of the model are provided below. The general concepts of the model are presented in Figure 1. Concrete is modelled as a two-phase composite that comprises a matrix (m) - representing the mortar- and spherical inclusions (Ω) - simulating the coarse aggregate particles. Additionally, penny-shaped cracks with various orientations and rough surfaces are distributed within the matrix phase. The elastic constitutive relationship for the two-phase composite was obtained by making use of the classic Eshelby inclusion solution and the Mori-Tanaka averaging method for a non-dilute distribution of inclusions:

$$\bar{\boldsymbol{\sigma}} = \mathbf{D}_{m\Omega} : (\bar{\boldsymbol{\varepsilon}} - \boldsymbol{\varepsilon}_a) \qquad (1)$$

where $\bar{\boldsymbol{\sigma}}$ and $\bar{\boldsymbol{\varepsilon}}$ are the average far-field stress and strain respectively. $\mathbf{D}_{m\Omega}$ is the elasticity tensor of the composite, $\mathbf{D}_{m\Omega} = \left(f_m \mathbf{D}_m + f_\Omega \mathbf{D}_\Omega \cdot \mathbf{T}_\Omega\right) \cdot \left(f_m \mathbf{I}^{4s} + f_\Omega \mathbf{T}_\Omega\right)^{-1}$ in which $\mathbf{D}_\beta$ represents the elasticity tensor and f_β the volume fraction of β-phase (β = m or Ω) with $f_m + f_\Omega = 1$. $\mathbf{I}^{4s}$ is the fourth order identity tensor and $\mathbf{T}_\Omega = \mathbf{I}^{4s} + \mathbf{S}_\Omega \cdot \left[\left(\mathbf{D}_\Omega - \mathbf{D}_m\right) \cdot \mathbf{S}_\Omega + \mathbf{D}_m\right]^{-1} \cdot \left(\mathbf{D}_m - \mathbf{D}_\Omega\right)$. $\mathbf{S}_\Omega$ is the Eshelby tensor for spherical inclusions [4].

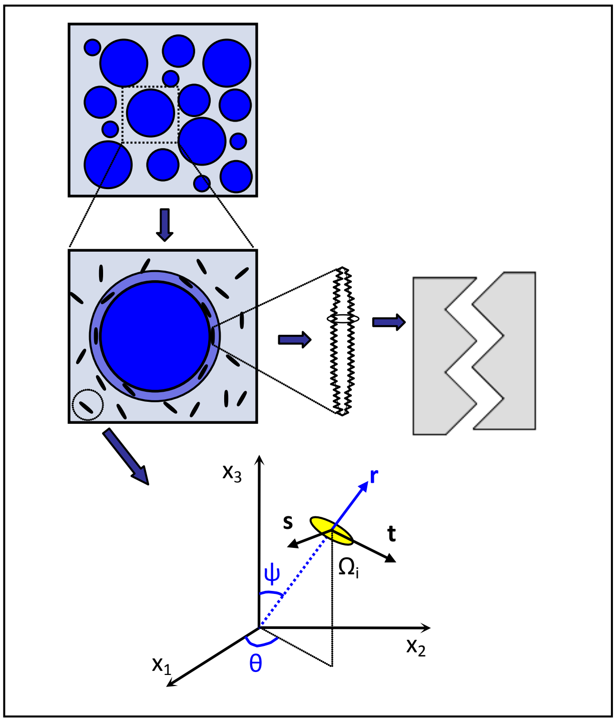

Figure 1: Model concepts.

Microcracking was addressed by evaluating the added strain $\boldsymbol{\varepsilon}_a$ from a series of penny-shaped microcracks distributed according to a crack density function $f(\theta,\psi)$. Employing Budiansky and O'Connell's solution [4], the added strain can be written as follows:

$$\boldsymbol{\varepsilon}_a = \left(\frac{1}{2\pi} \int_{2\pi} \int_{\frac{\pi}{2}} \mathbf{N}^T : \mathbf{C}_a : \mathbf{N}\, f(\theta,\psi)\, \sin(\psi) d\psi d\theta \right) : \bar{\boldsymbol{\sigma}} \qquad (2)$$

in which $\mathbf{C}_a$ is the local compliance tensor in the local coordinate system of a microcrack (r,s,t) and $\mathbf{N}$ the stress transformation tensor.

The crack density parameter may be related to a directional damage parameter ω ($0 \le \omega \le 1$) such that:

$$f(\theta,\psi)\,\mathbf{C}_a = \frac{\omega(\theta,\psi)}{1-\omega(\theta,\psi)}\mathbf{C}_{\mathrm{L}} = \mathbf{C}_{\alpha}(\theta,\psi) \quad (3)$$

where $\mathbf{C}_{\mathrm{L}} = \frac{1}{\mathrm{E}_{\mathrm{m}}}\begin{bmatrix} 1 & 0 & 0 \\ 0 & \frac{4}{2-\upsilon_{\mathrm{m}}} & 0 \\ 0 & 0 & \frac{4}{2-\upsilon_{\mathrm{m}}} \end{bmatrix}$ is the local elastic compliance tensor, with υ_m and E_m being the Poisson's ratio and the Young's modulus of the matrix phase respectively. Introducing Eq. (2) and Eq. (3) into Eq. (1) and rearranging gives:

$$\bar{\boldsymbol{\sigma}} = \left(\mathbf{I}^{4s} + \frac{\mathbf{D}_{\mathrm{m}\Omega}}{2\pi} \int_{2\pi}\int_{\frac{\pi}{2}} \mathbf{N}^{\mathrm{T}} : \mathbf{C}_{\alpha}(\theta,\psi) : \mathbf{N} \cdot \sin(\psi)\, d\psi\, d\theta \right)^{-1} \cdot$$
$$\cdot \mathbf{D}_{\mathrm{m}\Omega} : \bar{\boldsymbol{\varepsilon}} \quad (4)$$

Microcracks were assumed to initiate, based on experimental evidence, in the interfacial transition zone between aggregate particles and cement matrix. In order to model this mechanism a microcrack initiation criterion was formulated which makes use of an exterior point Eshelby solution that provides the expression of the total stress field outside an ellipsoidal inclusion embedded in an infinite elastic matrix [5]. The Mori-Tanaka averaging method was applied in order to account for the interaction between inclusions and the total stress field in the matrix outside an inclusion (for the composite) was obtained as:

$$\boldsymbol{\sigma}_{\mathrm{m}\Omega}(\mathbf{x}) = \mathbf{D}_{\mathrm{m}} \cdot \left[\mathbf{I}^{4s} + \mathbf{S}_{\mathrm{E}}(\mathbf{x}) \cdot \mathbf{B}_{\Omega} \right] \cdot \left[\mathrm{f}_{\Omega}\mathbf{T}_{\Omega} + \mathrm{f}_{\mathrm{m}}\mathbf{I}^{4s} \right]^{-1} :$$
$$: \left(\bar{\boldsymbol{\varepsilon}} - \boldsymbol{\varepsilon}_{\mathrm{a}} \right) \quad (5)$$

in which $\mathbf{B}_{\Omega} = -\left[\mathbf{S}_{\Omega} + \left(\mathbf{D}_{\Omega} - \mathbf{D}_{\mathrm{m}} \right)^{-1} \cdot \mathbf{D}_{\mathrm{m}} \right]^{-1}$. $\mathbf{S}_E(\mathbf{x})$ is the exterior point Eshelby tensor for spherical inclusions [6] and $\mathbf{x}$ is the position vector relative to the centre of inclusion. When the composite is subjected to uniaxial compressive stresses, the expression of the stress field in the matrix phase outside the inclusion in Eq. (5) captures sharp gradients and lateral tensile stress concentrations in a region adjacent to a matrix-inclusion interface. This enables the model to naturally simulate compressive splitting cracks. In each direction cracking is assumed to initiate when the local principal stress at the peak position in Eq. (4) reaches the tensile strength of the interface f_{ti}. The implementation of the microcrack initiation criterion into the constitutive model enables the use of realistic material properties in order to obtain a correct cross-cracking response, as shown in [1].

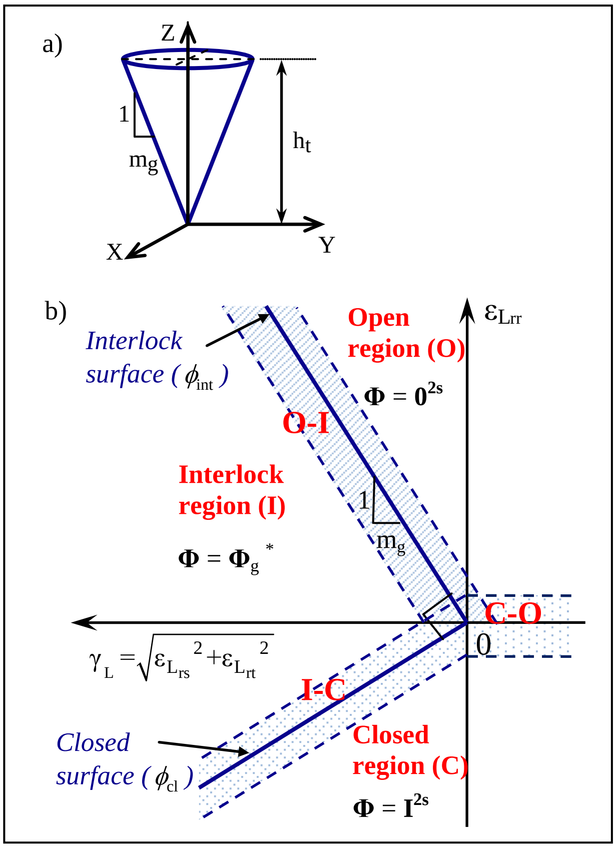

Figure 2: a) Schematic representation of a conical tooth b) Rough contact.

A rough crack closure component was then implemented to simulate the recovery of stress on microcracks that regain contact. In each direction the local stress was written as a summation of the average stress on intact material and the recovered stress on debonded material that regains contact.

$$\mathbf{s}_\alpha = (1-\omega)\mathbf{D}_L : \boldsymbol{\varepsilon}_L + H_f(\boldsymbol{\varepsilon}_L)\omega\mathbf{D}_L \cdot \boldsymbol{\Phi}(m_g, \boldsymbol{\varepsilon}_L) : \boldsymbol{\varepsilon}_L \quad (6)$$

H_f is a reduction function that decreases from 1 to 0 as the potential for shear transfer reduces with increasing crack opening. This is given by $H_f(\boldsymbol{\varepsilon}_L) = e^{-c_1 \frac{\varepsilon_{Lrr} - \varepsilon_{tm}}{\beta \cdot \varepsilon_0}}$ with $c_1 = 3$. Parameter β is the normalised asperity height, $\beta = h_t/u_0$, $\mathbf{D}_L = \mathbf{C}_L^{-1}$ and $\boldsymbol{\varepsilon}_L$ is the local strain tensor.

$\boldsymbol{\Phi}(m_g, \boldsymbol{\varepsilon}_L)$ is a contact matrix that depends upon the contact state -open, interlock or closed- as illustrated in Figure 2b.

Table 1: Unsmoothed contact formulation

Region	Contact state	Contact matrix
$\phi_{int}(\boldsymbol{\varepsilon}_L, m_g) \geq 0$	Open	$\boldsymbol{\Phi} = \mathbf{0}^{2s}$
$\phi_{int}(\boldsymbol{\varepsilon}_L, m_g) < 0$ and $\phi_{cl}(\boldsymbol{\varepsilon}_L, m_g) > 0$	Shear contact or interlock	$\boldsymbol{\Phi} = \boldsymbol{\Phi}_g$
$\phi_{cl}(\boldsymbol{\varepsilon}_L, m_g) \leq 0$	Closed	$\boldsymbol{\Phi} = \mathbf{I}^{2s}$

Where:

$$\boldsymbol{\Phi}_g = \frac{1}{1+m_g^2}\left(\left(\frac{\partial \phi_{int}}{\partial \boldsymbol{\varepsilon}_L}\right)\left(\frac{\partial \phi_{int}}{\partial \boldsymbol{\varepsilon}_L}\right)^T + \frac{\partial^2 \phi_{int}}{\partial \boldsymbol{\varepsilon}_L^2}\right) \quad (7)$$

and

$$\phi_{int}(\boldsymbol{\varepsilon}_L, m_g) = m_g \varepsilon_{Lrr} - \sqrt{\varepsilon_{Lrs}^2 + \varepsilon_{Lrt}^2}$$
$$\phi_{cl}(\boldsymbol{\varepsilon}_L, m_g) = \varepsilon_{Lrr} + m_g\sqrt{\varepsilon_{Lrs}^2 + \varepsilon_{Lrt}^2} \quad (8a,b)$$

m_g is the slope of the interlock contact surface and, in a physical sense, it represents the slope of the asperity (Figure 2a,b), thus being a measure of the crack surface roughness. Mihai and Jefferson [1] expanded the contact component to account for the variability of the crack roughness which gave the recovered stress as a summation:

$$\mathbf{s}_\alpha = \mathbf{D}_L \cdot \left[(1-\omega)\mathbf{I}^{2s} + \omega \cdot \sum_k p_k H_{fk} \boldsymbol{\Phi}_k\right] : \boldsymbol{\varepsilon}_L \quad (9)$$

The added compliance including contact $\mathbf{C}_{c\alpha}$, given in Eq. (10), is obtained by removing the elastic compliance from Eq. (9). Finally, $\mathbf{C}_\alpha = (\omega/(1\text{-}\omega))\mathbf{C}_L$ in Eq. (4) is replaced with $\mathbf{C}_{c\alpha}$ to give the final average stress – average strain relationship. The integration over a hemisphere in Eq. (4) is evaluated numerically by employing McLaren integration rule with 29 sample directions.

$$\mathbf{C}_{c\alpha} = \left[[(1-\omega)\mathbf{I}^{2s} + \omega \cdot \sum_k p_k H_{fk} \boldsymbol{\Phi}_k]^{-1} - \mathbf{I}^{2s}\right] \cdot \mathbf{C}_L \quad (10)$$

3 SMOOTHED CONTACT STATE FUNCTION

It was found that the use of discrete contact conditions can, under certain conditions, lead to spurious oscillatory response, which has been termed ‘chatter’ [7]. The present model can exhibit this type of behaviour - even in single point stress-strain simulations- when different contact conditions are active on different microcrack planes (Figure 3).

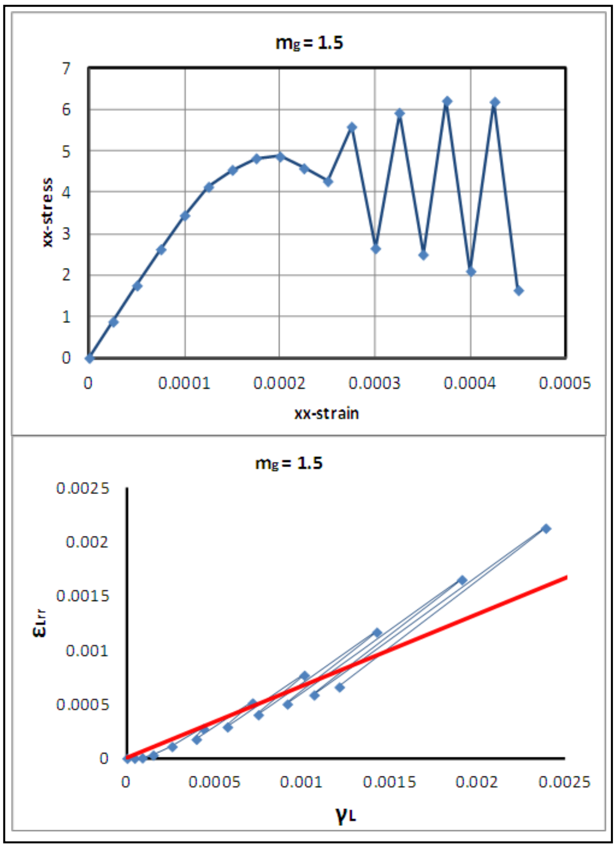

Figure 3: Examples of rough contact related chatter

To minimize the potential for spurious contact chatter behaviour at a constitutive level, a single smoothed expression, given in Eq. (11), which encompasses all three contact states, is proposed to replace the discrete contact formulation in Table 1:

$$\mathbf{\Phi}(\boldsymbol{\varepsilon}_L,\mathrm{m}_g)=\lambda_{cl}(\boldsymbol{\varepsilon}_L,\mathrm{m}_g)\cdot\mathbf{I}^{2s}+\left[1-\lambda_{cl}(\boldsymbol{\varepsilon}_L,\mathrm{m}_g)\right]\cdot \cdot\lambda_{int}(\boldsymbol{\varepsilon}_L,\mathrm{m}_g)\cdot\mathbf{\Phi}_g(\boldsymbol{\varepsilon}_L,\mathrm{m}_g) \quad (11)$$

in which $\lambda_*(\boldsymbol{\varepsilon}_L,\mathrm{m}_g), *=\text{'int'}\ \textit{or}\ \text{'cl'}$, are modified tanh type functions that interpolate between 0 and 1. In effect, three transition bands between each pair of contact regions are formed (Figure 2b) based on the smoothed contact formulation in Eq. (11). Each interpolation function features three dimensionless smoothing parameters that control the width of the transition bands, the slope of the interpolation function and the position of the transition band relative to the relevant contact surface respectively. The development of the interpolation functions λ as well as a parametric study based on which values were assigned to the three smoothing parameters, are fully detailed in a forthcoming publication [8].

4 NUMERICAL SIMULATIONS

The smoothed contact function in Eq. (11) was found to be effective at removing chatter and smoothing the response. This is illustrated in Figure 4 for a single component contact formulation.

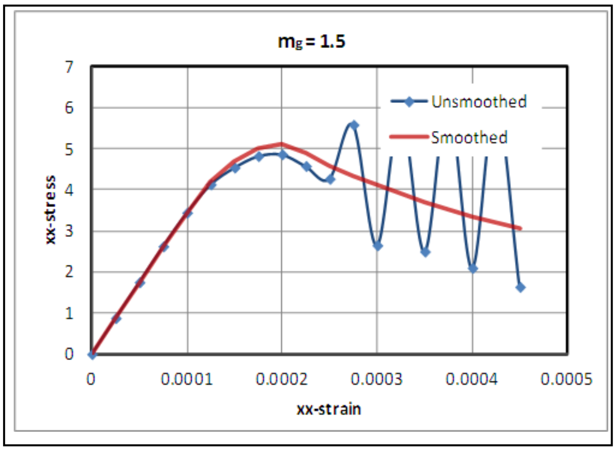

Figure 4: Uniaxial compression predictions for unsmoothed and smoothed contact

The performance of the smoothed contact function is investigated in detail for uniaxial compression and uniaxial tension cases in Reference [8]. In the present work, further study of the performance of the micromechanical constitutive model with smoothed contact in combined tension and compression multiaxial loading is presented. Biaxial simulations were carried out with the unsmoothed contact (U) and smoothed contact (S) versions of the model using the material properties in Table 2 and the contact components from a Gamma probability density function detailed in [8]. Compressive strains were prescribed along the xx direction and tensile strains were prescribed along the yy direction. The predicted stress – strain responses along the two orthogonal loading directions are presented in Figures 5 and 6.

It can be observed that the smoothed contact formulation performs well and is efficient in smoothing the response in combined tension and compression loading cases.

Table 2: Material properties

E_m MPa	E_Ω MPa	υ_m	υ_Ω	f_{ti} MPa	u_0 mm	d_{max} mm
31000	55000	0.19	0.21	1.0	0.1	10

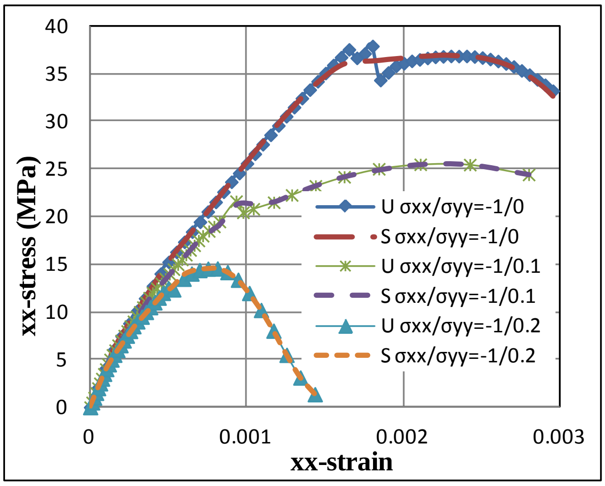

Figure 5: Numerical predictions for unsmoothed and smoothed contact (compression)

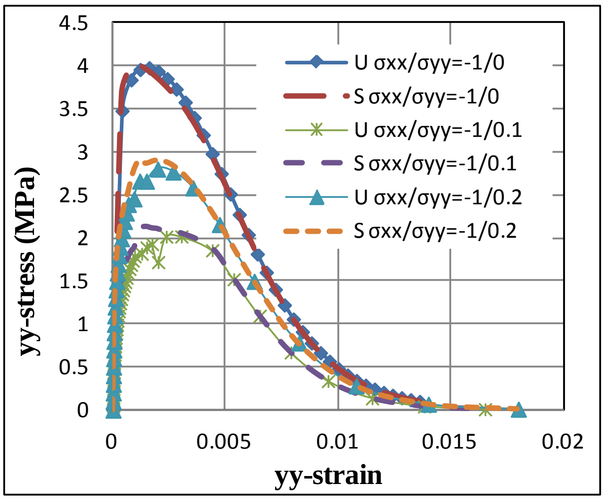

Figure 6: Numerical predictions for unsmoothed and smoothed contact (tension)

Numerical results for a uniaxial compression strain path obtained with the micromechanical model and using realistic material data detailed in [1] are presented in Figure 7. Good correlation with experimental data indicates that the proposed model captures key characteristics of the overall macroscopic behaviour.

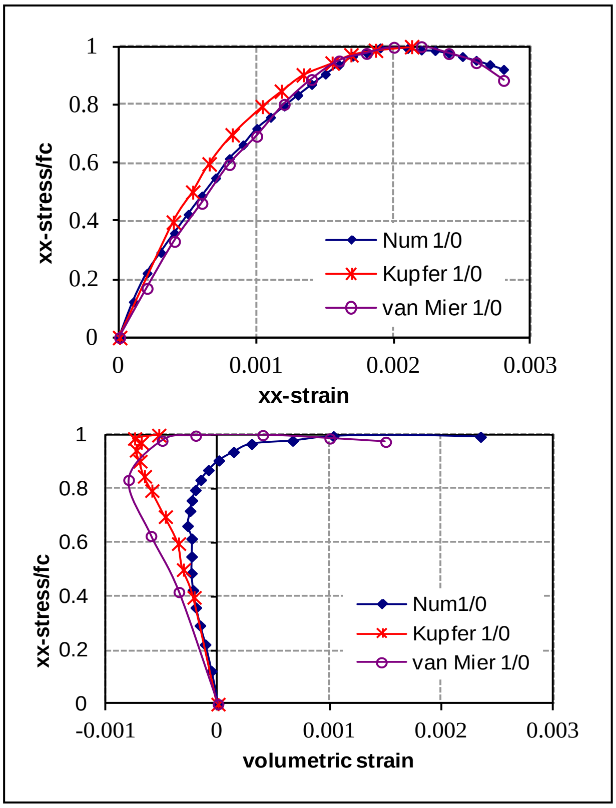

Figure 7: Uniaxial compression response (compression +ve)

5 CONCLUSIONS

The micromechanical model is able to simulate successfully micromechanisms that lead to failure while employing realistic and meaningful material parameters. A smoothed contact state function was proposed and found to be effective in removing spurious chatter behaviour.

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