Non-local micromechanical anisotropic damage modeling for quasi-brittle materials: formulation and implementation

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ABSTRACT: A nonlocal anisotropic damage model is proposed for quasi-brittle materials, such as concrete and rock. The local anisotropic damage model is formulated by combining a free energy derived from micromechanics with phenomenological yield criteria and damage potentials. The trace of the total strain is used to distinguish tensile and compressive loading paths, and to account for the influence of the confining pressure on the propagation of compression cracks. Yield criteria in tension and compression are expressed in terms of equivalent strains, which depend on the difference between principal strain components. A non-local measure of strain is used to avoid localization. Constitutive parameters are calibrated against published experimental data for concrete and shale. Simulations of three-point bending tests show that non-local enhancement is necessary and efficient to avoid mesh dependency upon strain softening. Simulations of borehole excavation damage zone show that the damage model is not mesh dependent upon stress hardening. Numerical predictions are in agreement with experimental observations and the model can capture unilateral effects, tensile softening, compressive hardening and confinement dependent compressive behavior.

1. INTRODUCTION

It is still a challenge to formulate a constitutive model that captures damage induced anisotropy and stiffness reduction, unilateral effects due to crack closure and a transition from brittle to ductile behavior at increasing confining stress (Krajcinovic et al., 1991; Chiarelli et al., 2003). What is the most appropriate way to express the free energy so that the direction dependence of crack inception and propagation can be captured? How to define the anisotropic damage variable to ensure straightforward physical interpretation and efficient computation: a second order or fourth order damage tensor (Leckie et al., 1981), or discrete crack densities (Jin & Arson, 2017)? How to address the salient material behavior differences between compressive and tensile loading (Lubarda et al., 1994; Comi & Perego, 2001)? In the case of strain softening behavior, what are the best techniques to regularize localization problems: the crack band theory (Bazant & Oh, 1983), the strain gradient (Geers et al., 1998) or an integration based nonlocal approach (Pijaudier-Cabot & Bazant, 1987)?

State-of-the-Art damage models are based on phenomenological or micromechanical approaches. In Continuum Damage Mechanics (CDM), the free energy, damage criteria and damage potentials are constructed in order to ensure thermodynamics consistency of the phenomenological model (Jin et al., 2017; Dragon et al., 2000). CDM models require a large number of constitutive parameters to be physically realistic and account for multiple phenomena. In micromechanics, fracture mechanics are used within a homogenization scheme, which ensures that the model provides physical predictions (Zhao et al., 2016; Zhu et al., 2008). However, convergence issues arise when implementing micromechanical models into Finite Element (FE) codes. Both phenomenological and micromechanical models with strain softening exhibit failure localization and mesh dependency. In this paper, we first formulate an anisotropic damage model by combining a free energy derived from micromechanics with phenomenological yield criteria and damage potentials. A non-local measure of strain is used to avoid localization. Finite Element simulations of three-point bending and borehole wall damage development are presented.

2. ANISOTROPIC DAMAGE MODEL

2.1. Constitutive equations

We assume that the material under study is populated with non-interacting cracks. The free enthalpy of a crack inclusion-matrix system as shown in Figure 1 is obtained by superposing the tensile and shear stresses that apply at crack surfaces (Budiansky & O’connell, 1976), and using a dilute homogenization scheme, by assuming arbitrary crack orientation (Shao et al., 1999). Stresses at crack faces are obtained by considering penny-shaped...
cracks embedded in an infinite matrix. The free energy is expressed as:

$$G(\sigma, \Omega) = \frac{1}{2} \sigma : S_0 : \sigma + a_1 \text{Tr}(\Omega \sigma)^2 + a_2 \text{Tr}(\sigma \cdot \Omega + \Omega \cdot \sigma)$$

$$+ a_3 \text{Tr}(\sigma \cdot \Omega \sigma) + a_4 \text{Tr}(\sigma \cdot \sigma)$$

(1)

Where $\Omega$ is the second order damage tensor, and

$$a_1 = -\frac{\mu}{140} c_1, \quad a_2 = \frac{7 + 2\mu}{14} c_1,$$

$$a_3 = \frac{\mu}{14} c_1, \quad a_4 = -\frac{\mu}{70} c_1,$$

$$c_1 = \frac{32}{3} \frac{1-\nu^2}{(2-\nu)E}$$

(2)

Note: $\mu = -\nu_0$ for open cracks and $\mu = -2$ for closed cracks.

The volumetric strain convention, the tensile evolution law is used. When the volumetric strain is negative (dilation with the soil mechanics soil sign convention), the tensile evolution law is used. For the case when all strain components are negative:

$$\Delta \epsilon^t = \epsilon^t_{eq} = (\kappa_t + a_t \text{Tr} \Omega)$$

$$\Delta \epsilon^c = \epsilon^c_{eq} + \eta \text{Tr} \epsilon - (\kappa_c + a_c \text{Tr} \Omega)$$

(5)

The trace of strain added in the expression of the compressive damage function allows accounting for the brittle-ductile transition at increasing confining pressure. Damage potentials are proposed to derive the damage rate in an explicit form. For tensile loading:

$$\dot{\Omega}_t = \dot{\lambda}_t D_t = \frac{\dot{\lambda}_t}{(\epsilon^t_{eq})^2} \begin{bmatrix} \langle \epsilon_1 \rangle^2 & 0 & 0 \\ 0 & \langle \epsilon_2 \rangle^2 & 0 \\ 0 & 0 & \langle \epsilon_3 \rangle^2 \end{bmatrix}$$

(6)

For compressive loading:

$$\dot{\Omega}_c = \dot{\lambda}_c D_c = \frac{\dot{\lambda}_c}{(\epsilon^c_{eq})^2} \begin{bmatrix} \langle \epsilon_1 \rangle^2 & 0 & 0 \\ 0 & \langle \epsilon_2 \rangle^2 & 0 \\ 0 & 0 & \langle \epsilon_3 \rangle^2 \end{bmatrix}$$

(7)

In which the Lagrange multiplier $\dot{\lambda}$ is determined from the consistency conditions that apply to the damage criteria in Eq. (5) The expression of the damage rate in Eq. (6) and Eq. (7) is chosen to ensure that the damage pattern follows experimental observations (Halm & Dragon, 1998). For example, a uniaxial tensile loading in direction 1 will only result in cracks perpendicular to the loading direction1, i.e. damage in direction 1: $\dot{\epsilon}_1^{eq} = \dot{\epsilon}_1 > 0$. A triaxial compression test with a loading axis parallel to direction 1 results in lateral damage even for the case when all strain components are negative: $\dot{\epsilon}_c^{eq} = \sqrt{\dot{\epsilon}_2} = \sqrt{\dot{\epsilon}_3} > 0$.

The consistency condition for the compressive damage function is expressed as:

$$0 = \frac{\partial f_c}{\partial \epsilon^c_{eq}} d\epsilon^c_{eq} + \frac{\partial f_c}{\partial \text{Tr} \epsilon} d\text{Tr} \epsilon + \frac{\partial f_c}{\partial \Omega} d\Omega \Rightarrow \epsilon^c_{eq} + \eta \delta : d\epsilon - \alpha_c \delta : \dot{\Omega}$$

(8)

Substitute the compressive flow rule of Eq. (7) into above, we obtain the expression of Lagrange multiplier as
\[ \dot{\lambda}_c = \frac{\varepsilon_{eq} \eta \delta : \varepsilon}{\alpha_c} \]  

Note that from Eq. (7), we have: \( \alpha_c \delta : \dot{\Omega} = \alpha_c \dot{\lambda}_c \). Similarly, we obtain the tensile Lagrange multiplier as

\[ \dot{\lambda}_t = \frac{\varepsilon_{eq}}{\alpha_t} \]  

2.2. Single element simulation in Abaqus

We implemented the proposed model in Abaqus UMAT and performed a series of simulations to test the ability of the model to capture unilateral effects, tensile softening, compressive hardening and confinement dependent compressive behavior. A linear cubic element is used. The orders of magnitude of the constitutive parameters are typical of concrete or rock (Table 1).

Figure 1 shows the results obtained during cyclic uniaxial tension and compression, simulated by fixing the vertical displacement (direction 1) of the 4 nodes on one face, and by applying positive and negative vertical displacements on the opposite face. Note that one of the nodes is fixed in all three directions to prevent free body rotation and movement. Damage, stress and strains are extracted from the 8 Gauss points. The constitutive model predicts softening after the tensile strength is reached. Only damage component develops, along the loading direction. When the damaged material is unloaded and further loaded in compression, the reduced tensile modulus recovers its original value before damage, while the damage value keeps constant. This is due to the closure of open mode I cracks generated in tension, which is called unilateral effect. When the element is reloaded in tension, cracks produced during the first loading cycle re-open, therefore the Young’s modulus abruptly changes from a non-damaged to damaged value. Once the stress level reaches the previous threshold, damage propagates further and the Young’s modulus decreases. Note that the constitutive laws are derived from micromechanics: damage presents crack density instead of a phenomenological stiffness reduction percentage, so damage can exceed 1.

Table 1. Material parameters used for the single element simulation in Abaqus

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<tr>
<td>( \eta )</td>
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Figure 2 shows the stress-strain curve and damage principal components during a test comprising uniaxial tensile loading, uniaxial compression, and tensile reloading. Note: the average value of damage, stress and strain obtained at the 8 Gauss points of the linear cubic element are used to plot the Figure.

Figure 3 shows the stress-strain curve and damage component evolution for a uniaxial compression test.

Figure 4 shows the deviatoric stress/strain curve for triaxial compression tests with confinements of 0 MPa and 5 MPa. The volumetric term added in Eq. (5) clearly allows capturing the increase of compressive strength with increased confinement.
usually a normalization coefficient used by where parameter (discussed by replaced by be done on strain, stress or inte each node, thus, the internal state variables not only (strain gradient method) are treated as additional degrees of freedom on each node, thus, the internal state variables not only depend on the nodal values of stress and strain, but also on their gradient. Gradient or integration enrichment can be done on strain, stress or internal variables (damage in this case). In the proposed model, the internal state variable $\varepsilon^{eq}$, which is used to calculate damage, is replaced by a nonlocal state variable $\varepsilon^{eq}$. It is calculated by spatial averaging over representative neighborhood (volume $V$), which depends on an internal length parameter (discussed later):

$$
\varepsilon^{eq}_i(x) = \int_{V} \beta(x, \xi) \varepsilon^{eq} (\xi) dV(\xi) \tag{11}
$$

where $i = c, t$ stands for compression, tension and $\alpha_0 (x, \xi)$ is the chosen weight averaging operator given by

$$
\beta(x, \xi) = \frac{\alpha(x, \xi)}{\Omega_r}
$$

$$
\Omega_r = \int_{V} \alpha(x, \xi) dV(\xi) \tag{12}
$$

$\Omega_r$ is the interaction volume at point $x$: it is the normalization coefficient used to preserve partition of unity. $\alpha(x, \xi)$ is the basic nonlocal weighting function, usually a Gaussian function or a bell-shape function. We use a bell-shape function (Figure 5):

$$
\alpha(r) = (1 - r^2/R^2)^2 . \tag{13}
$$

where $r = \|x - \xi\|$ is the distance between the (local) point $x$ and points in the neighborhood. $\xi = 0$ if $x < 0$, $\xi = x$ if $x \geq 0$. $R$ is the radius of the nonlocal influence zone, also called characteristic internal length. The value of $R$ is about 2-3 times the size of the largest inhomogeneity in the material under study.

Fig. 4. Deviatoric stress-strain curve and damage evolution for a triaxial compression test at different levels of confinement. Note the lateral damage components are equal $\Omega_2 = \Omega_3$, so only $\Omega_2$ is shown in this plot.

2.3. Nonlocal enrichment

In a strain softening material, the extent of the damaged zone is mesh-dependent. The amount of energy required to create a unit area of fracture does not converge upon mesh refinement. A number of numerical techniques were proposed to solve this localization issue, mainly the strain gradient approach and the integration based nonlocal approach (Pijaudier-Cabot and Bazant, 1987). In the strain gradient method, the displacement gradient (strain) are treated as additional degrees of freedom on each node, thus, the internal state variables not only depend on the nodal values of stress and strain, but also on their gradient. Gradient or integration enrichment can be done on strain, stress or internal variables (damage in this case). In the proposed model, the internal state variable $\varepsilon^{eq}$, which is used to calculate damage, is replaced by a nonlocal state variable $\varepsilon^{eq}$. It is calculated by spatial averaging over representative neighborhood (volume $V$), which depends on an internal length parameter (discussed later):

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\varepsilon^{eq}_i(x) = \int_{V} \beta(x, \xi) \varepsilon^{eq} (\xi) dV(\xi) \tag{11}
$$

where $i = c, t$ stands for compression, tension and $\alpha_0 (x, \xi)$ is the chosen weight averaging operator given by

$$
\beta(x, \xi) = \frac{\alpha(x, \xi)}{\Omega_r}
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$\Omega_r$ is the interaction volume at point $x$: it is the normalization coefficient used to preserve partition of unity. $\alpha(x, \xi)$ is the basic nonlocal weighting function, usually a Gaussian function or a bell-shape function. We use a bell-shape function (Figure 5):

$$
\alpha(r) = (1 - r^2/R^2)^2 . \tag{13}
$$

where $r = \|x - \xi\|$ is the distance between the (local) point $x$ and points in the neighborhood. $\xi = 0$ if $x < 0$, $\xi = x$ if $x \geq 0$. $R$ is the radius of the nonlocal influence zone, also called characteristic internal length. The value of $R$ is about 2-3 times the size of the largest inhomogeneity in the material under study.

Fig. 5. Bell-shape weight function used in the non-local model, with R=0.02.

In finite element analysis, the non-local equivalent strain can be calculated by using the weighted average of the equivalent strain obtained locally at each Gauss Point, as follows (De Vree et al., 1995):

$$
\varepsilon^{eq} = \frac{1}{\sum_{ip}^{nip} \alpha_{ip} \Delta V_{ip}} \sum_{ip}^{nip} \alpha_{ip} \Delta V_{ip} \varepsilon_{ip}^{eq} \tag{14}
$$

In which index $ip$ refers to an integration point in a set of surrounding Gauss points, and $nip$ is the total number of Gauss points in that set. $\Delta V_{ip}$ is the integration volume associated with Gauss point $ip$. $\alpha_{ip}$ is the weight determined from the distance $r$ between the (local) point $x$ and integration point $ip$.

3. NUMERICAL SIMULATION

3.1. Calibration of tensile parameters for concrete

We calibrated the proposed damage model against a stress/strain curve obtained by Bazant and Pijaudier-Cabot (1989) during uniaxial tensile test performed on concrete. Because uniaxial tensile test usually results in a highly localized macro fracture, the stress strain recorded cannot truly reflect the behavior of the material considered as a continuum, because strain is not uniform throughout the sample. Therefore, concrete was glued to a thin sheet of steel placed parallel to the loading axis. A dedicated MATLAB code employing the Interior Point Algorithm was adopted to minimize the residual
between experimental results and numerical predictions. In this algorithm, we supply an initial guess for the parameters that need to be calibrated and bound constraints for each parameter. The algorithm calculates gradients to search for local minima. The results of the calibration are reported in Table 2. Only the axial strain is available in the experimental dataset. The other strain components do not contribute to damage development, so we calculate equivalent strains and damage from the axial strain only. After the stiffness matrix is determined, the lateral zero stress condition is utilized to obtain lateral strain components (Figure 6).

Table 2. Material tensile parameters calibrated for concrete.

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<td>$4.74 \times 10^{-4}$</td>
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3.2. Three-point bending test

In order to demonstrate the capability of the proposed non-local damage model to predict the softening behavior of brittle solids and eliminate mesh dependency, we simulated the classical three-point bending test with the parameters calibrated for concrete (Table 2). The specimen geometry, notch size and boundary conditions are shown in Figure 7. Triangular elements with two mesh densities are used.

Fig. 7. Mesh density, geometry and boundary conditions for the simulated three-point bending test. Top: fine mesh. Bottom: coarse mesh.

(b) Nonlocal damage model, coarse mesh

Fig. 6. Calibration of the proposed non-local damage model against uniaxial tension experimental data (Bazant and Pijaudier-Cabot, 1989)

(a) Stress-strain curve

(b) Damage components evolution
3.3. Calibration of compressive parameters for shale

As demonstrated in the single element simulation, the proposed damage model can only capture the pre-peak stress hardening in compression, because crack coalescence is ignored in the model. Correspondingly, we only use the prepeak stress-strain experimental data obtained during a triaxial compression test carried on Bakken shale samples to calibrate the model (Amendt et al., 2013). Like in the previous case, the calibration process is essentially an optimization problem with bounding constraints on material parameters. However, by contrast with the uniaxial test, all three strain components play a role to determine damage evolution. So we cannot directly supply strain components to obtain stress counterparts, because the predicted confinement varies with damage evolution. As a result, we use stress as input and an iteration scheme to update the corresponding strains. We adopt a cutting plane algorithm, which is a type of return mapping algorithm, to maintain the stress-strain state on the damage surface after yielding.

First, we obtain the total strain increment by differentiating the constitutive relationship as follows:

\[ \epsilon = \mathcal{S}(\Omega): \sigma \]

\[ d\epsilon = \mathcal{S}(\Omega): d\sigma + \sigma: \partial_n \mathcal{S}: d\Omega \]

We linearize the yield function around the current values of variables, \( \epsilon^{i+1}_{n+1}, \Omega^{i+1}_{n+1} \), as

\[ f^{i+1}_{n+1} \approx f^{i}_{n+1} + \partial f^{i}_{n+1} \cdot [\epsilon^{i+1}_{n+1} - \epsilon^{i}_{n+1}] + \partial \Omega^{i+1}_{n+1} \cdot [\Omega^{i+1}_{n+1} - \Omega^{i}_{n+1}] \]  

After discretizing the strain and damage tensors, we use the flow rule to get:

\[ \epsilon^{i+1}_{n+1} - \epsilon^{i}_{n+1} = -\Delta \lambda^{i}_{n+1} \left[ \sigma^{i}_{n+1} : \partial \Omega^{i}_{n+1} : \mathbf{D}_\epsilon \right] \]

\[ \Omega^{i+1}_{n+1} - \Omega^{i}_{n+1} = -\Delta \lambda^{i}_{n+1} \mathbf{D}_\epsilon \]

After substituting Eq. (18) into Eq. (17), we obtain the Lagrange multiplier

\[ \Delta \lambda^{i}_{n+1} = -\frac{f^{i+1}_{n+1}}{\partial \epsilon^{i+1}_{n+1} : \sigma^{i+1}_{n+1} : \partial \Omega^{i+1}_{n+1} : \mathbf{D}_\epsilon - \partial \Omega^{i+1}_{n+1} : \mathbf{D}_\epsilon} \]

The specific steps of the resolution algorithm are the following:

1. For a given stress increment, assume no damage growth, use the previous converged compliance tensor and compute the strain increment.

Figure 8 shows the distribution of damage, computed for the two different meshes, with or without nonlocal enhancement. In the nonlocal computations, the characteristic internal length \( R \) is set to 0.01m. All simulations yield mode I vertical cracks (horizontal damage), which is conform to the expectations. The local damage model provides mesh dependent results (Figure 8(a) and 8(c)). The failure process zone clearly depends on mesh size, which implies that if further mesh refinement had been done, a very small failure process zone with insignificant dissipation energy would have been obtained – which is not physically reasonable. By contrast, mesh dependence is avoided when the nonlocal damage model is used (Figure 8(b) and 8(d)). Note that the use of the dilute homogenization scheme makes it impossible to account for crack interactions and coalescence, and therefore limits the application of the model to failure analysis. The proposed non-local damage model can capture crack initiation and propagation, and can be coupled to a macroscopic fracture model (e.g. Cohesive Zone Model or XFEM) to capture also the initiation of crack coalescence.
(2) Check yield criteria: if the yield function is less than 0, then exit. Otherwise, go to (3).

(3) Use Eq. (19) to compute the Lagrange multiplier.

(4) Update the strain and damage tensors, go to (2).

After utilizing the return mapping and interior point algorithms, we obtain the calibrated material compressive parameters, listed in Table 3.

Table 3. Material compressive parameters calibrated for shale.

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<tr>
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Figure 9 shows the results obtained after model calibration for three confining pressures: $\sigma_c = 6.9$, 13.8 & 20.7 MPa. The damage model predictions satisfactorily match the experimental data, especially for the simulation at a confinement of 13.8 MPa (used for model validation). The discrepancy observed for the lateral strains is due to the fact that shale deforms inelastically during the test, while the proposed model is hyper-elastic before damage initiation. From the damage evolution shown in Figure 9(b), the confinement dependent compressive behavior is well captured: higher deviatoric stress is required for yielding. Only lateral damage components have a positive value, which is consistent with experimental observations.

3.4. Excavation damage zone around a borehole

Fig. 10. Geometry and boundary conditions of the borehole simulation

(a) Triaxial stress-strain curves

(b) Evolution of damage components in triaxial tests

Fig. 9. Calibration and validation of the proposed non-local damage model against experimental stress-strain curves obtained from triaxial compression tests performed on shale, under various confining pressure.
We carried out simulations on the development of the excavation damage zone around a borehole. We used the constitutive material parameters calibrated for shale (Table 3). The problem geometry and boundary conditions are shown in Figure 10. Two types of meshes with plane strain triangular elements are used. Figure 11 shows the distributions of vertical and horizontal damage obtained with the coarse and fine meshes. No mesh dependence was noted with the local damage model presented in Section 2.1 because the loading is purely compressive. As a result, we present the results obtained with both meshes for the local damage model only. The damage distribution matches the distribution of maximum compressive stress, obtained in the vertical direction, which is conform to field observations.

4. CONCLUSION

We propose a nonlocal micromechanics based anisotropic damage model for brittle geomaterials. The Gibbs energy is obtained by using a dilute homogenization scheme. Two distinct damage criteria are used for tension and compression, based on positive strains and deviatoric strain components, respectively. Damage functions are expressed in terms of equivalent strains and damage evolution laws are obtained from damage potentials. Single element Finite Element simulations of uniaxial tension, uniaxial compression and triaxial compression demonstrate that the proposed model captures nonlinear stress strain behaviour with damage induced stiffness anisotropy, loading path-dependent strain softening/hardening, unilateral effects due to crack closure and the brittle-ductile transition, which depends on the confining pressure. We further enhance the model with nonlocal equivalent strains, which depend on n internal length parameter. We calibrate the non-local damage parameters against published experimental data for concrete and shale. Simulations of three-point bending tests show that non-local enhancement is necessary and efficient to avoid mesh dependency upon strain softening. Simulations of borehole excavation damage zone show that the damage model is not mesh dependent upon stress hardening. Numerical predictions are in agreement with experimental observations and the model can capture unilateral effects, tensile softening, compressive hardening and confinement dependent compressive behavior.

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