A Model for Predicting Damage Dependent Response of Inelastic Media with Microstructure

by

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Abstract

This paper presents a model developed for predicting the mechanical response of inelastic media with heterogeneous microstructure. Particular emphasis is given to the development of microstructural damage along grains. The model is developed within the concepts of continuum mechanics, with special emphasis on the development of internal boundaries in the continuum by utilizing fracture mechanics-based cohesive zone models. In addition, the grains are assumed to be characterized by nonlinear viscoplastic material behavior. Implementation of the model to a finite element computational algorithm is also briefly described, and example solutions are obtained. Finally, homogenization procedures are discussed for obtaining macroscopic damage dependent mechanical constitutive equations that may then be utilized to construct a well-posed boundary value problem for the macroscopically homogenized damage dependent medium.
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Introduction

Geologic media such as rock salt demonstrate a significant amount of heterogeneity when viewed on a scale at which individual grains can be observed, as shown in Figure 1. However, when modeling the mechanical response of an object that is large compared to the scale of the grains, it is generally intractable, and indeed usually unnecessary from the standpoint of engineering accuracy, to model the heterogeneity associated with each grain. In this case, it is often assumed that the object may be considered to be macroscopically homogeneous. The construction of a model based on this assumption is quite straightforward if the medium in question does not dissipate energy. However, when energy dissipation does occur because of molecular scale phenomena such as dislocation propagation and/or fracture mechanisms including grain boundary sliding, the process of posing a homogeneous constitutive model for the macroscopic medium can be quite cumbersome.

One approach to the construction of the homogenized macroscopic constitutive model is to perform experiments on specimens that are large compared to the asperities, but this can be very expensive and time consuming. An alternative is to pose a micromechanics model that accounts for the heterogeneity and then homogenize by some consistent means the solution to this problem. While this approach may also be complicated, there are numerous advantages [1, 2]. One advantage is that by using micromechanics only the behavior of the constituents, which may be isotropic, needs to be evaluated, even though the macroscopic behavior may be orthotropic. Another advantage is that the micromechanics solutions will give macroscopic properties that apply for any mixture of volume fractions of constituents.

Essentially, the solution to the global problem will require the following three steps to be completed: (1) formulation and solution of a heterogeneous micromechanics problem, (2) homogenization of the micromechanics solution to produce a macroscopic constitutive model, and (3) formulation and solution of a homogeneous macromechanics problem. These will be discussed in the succeeding sections.

Formulation and Solution of the Micromechanics Problem

Consider the heterogeneous body with volume $V$ and boundary $\partial V$, shown in Figure 1. We assume that this volume $V$ is small compared to the volume of the part of interest, $V_G$, and large compared to the volume of a typical grain. The following model is proposed for predicting the mechanical state in $V + \partial V$:

(1) Equilibrium Equations:

$$\sigma_{ij,j} = 0 \quad \text{in} \quad V$$

(2) Boundary Conditions:

$$T_i = \sigma_{ij} n_j \quad \text{on} \quad \partial V$$

where $\sigma_{ij}$ is the symmetric stress tensor, and $T_i$ is the traction vector. Here $j$ denotes differentiation with respect to the local coordinates $x_j$. 


Figure 1. A continuum with heterogeneous microstructure.
(2) Strain-displacement Relations:

\[ \varepsilon_{ij} = \frac{1}{2} (\mathbf{u}_i, \mathbf{u}_j) \quad \text{in} \quad V \]  

(3) Constitutive Behavior:

\[ \varepsilon_{ij} = C_{ijkl} \sigma_{kl} + \varepsilon_{ij}^l \]  

where \( C_{ijkl} \) is the linear elastic (constant) compliance tensor, and \( \varepsilon_{ij}^l \) is the inelastic strain tensor governed by an evolution law of the form:

\[ \dot{\varepsilon}_{ij} = \Omega_{ij} \left( \sigma_{kl}, \varepsilon_{ij}^l, \alpha_{kl}^\mu \right) \quad \mu = 1, \ldots, n \]  

where \( \alpha_{kl}^\mu \) is a set of internal variables governed by evolution laws of the form:

\[ \dot{\alpha}_{kl}^\mu = \Phi_{kl}^\mu \left( \sigma_{kl}, \varepsilon_{ij}^l, \alpha_{kl}^\mu \right) \quad \eta, \mu = 1, \ldots, n \]  

where \( n \) is the number of internal variables. In the case of salt, the precise form of Equations 5 and 6 is modeled herein by the Munson-Dawson model [3]. Furthermore, in the undeformed state, the salt is assumed to be statistically isotropic, so that:

\[ C_{ijkl} = \frac{1}{3} \left( C_2 - C_1 \right) \delta_{ij} \delta_{kl} + \frac{1}{2} C_1 \left( \delta_{ik} \delta_{jl} + \delta_{il} \delta_{jk} \right) \]  

(4) Cohesive Zone Model:

Finally, there is assumed to be a set of planes of zero initial volume in \( V \) denoted \( \partial V_f \) with constitutive behavior governed by the Tvergaard cohesive zone model with a traction-displacement relation given by [4] (for the two-dimensional case):
where $T_n$, $T_s$, and $u_n$, $u_s$ are the normal and shear components of tractions and relative displacements, respectively, on a $\partial V_j$. Furthermore,

$$T_n = \frac{27}{4} \sigma_{\text{max}} \frac{u_n}{\delta_n} (1 - 2\lambda + \lambda^2)$$

$$T_s = \alpha_s \frac{27}{4} \sigma_{\text{max}} \frac{u_s}{\delta_s} (1 - 2\lambda + \lambda^2)$$

(9)

and $\sigma_{\text{max}}$, $\delta_n$, $\delta_s$, and $\alpha_s$ are material constants for the cohesive zone. There are additional constraints on $T_n$ and $T_s$ such that unloading is linear in $u_n$ and $u_s$, respectively, and if $\delta^2 = 1$,

$$T_n = T_s = 0.$$}

The above cohesive zone model has the net effect that when the critical value of $\lambda = 1$ is reached, internal traction-free boundaries are produced anywhere in the micromechanical problem that cohesive zones are placed. In this paper, cohesive zones will be placed along all grain boundaries.

The first author and coworkers have shown in recent research [5,6] that the above cohesive zone model is consistent with the concept of a Griffith energy criterion for crack extension as follows [7]:

$$G \geq G_{cr} \Rightarrow \frac{d}{dt} (\partial V_j) \geq 0$$

(11)

where $G$ is the available energy release rate for crack extension and $G_{cr}$ is the barrier that must be overcome for crack extension to occur. Due to the nature of the Tvergaard model, $G_{cr}$ is a material constant in the present paper for the case of self-similar crack growth. This is not always the case in inelastic media and may well be an oversimplification in salt. A more advanced cohesive zone model in which $G_{cr}$ is not a constant may well be warranted. One such possibility is currently under investigation by the first author and coworkers [8].

The above equations, together with appropriate boundary conditions on $\partial V$, constitute a well-posed boundary value problem that is solved on a DEC 3500S AXP computer with the finite element code SPECTROM-32 (version 4.10) [9]. The discretization and implementation of this model into a finite element code are briefly described in Reference 10.

**Homogenization of the Micromechanics Solution**

For purposes of analyzing large-scale continua with spatially variable displacements, it is inconvenient to model each grain boundary with a cohesive zone. If the average grain diameter, $d_g$, is small compared to the scale of the continuum of interest, $d_c$ ($d_g << d_c$), and the large-scale...
problem is statistically homogeneous, then it is usually sufficiently accurate to model the macroscopic problem with volume $V_G$ and boundary $\partial V_G$ as if the material were homogeneous and simply connected (at least until damage becomes so widespread that the crack lengths are comparable to the dimension of the body of interest). Assuming that the analysis of the $V + \partial V$ is also statistically homogeneous, then the solution to this problem can be homogenized to produce the macroscopically homogeneous constitutive model to be utilized in the large-scale analysis. This can be accomplished by volume averaging the solution to the micromechanics problem. Therefore, we first introduce the following notation for a generic function $f(x, t)$:[1, 11, 12]:

$$\bar{f}(\bar{x}_G, t) \equiv \frac{1}{V_{\bar{x}_G}} \int f(\bar{x}, t) dV$$

where $\bar{x}$ represents the local coordinated system utilized in the micromechanics solution, and $\bar{x}_G$ is the global coordinate system used in the macromechanical problem, as shown in Figure 1.

Suppose that in the present case the external boundary, $\partial V_E$, of the micromechanical problem is subjected to spatially homogeneous tractions such that:

$$T_i = \Sigma_q n_j \quad \text{on} \quad \partial V_E \quad (13)$$

where $\Sigma_q$ are spatially constant on the boundary $\partial V_E$. Furthermore, one can define the boundary averaged strains as follows:

$$E_{ij} \equiv \frac{1}{V_{\partial V_E}} \int \frac{1}{2}(u_i n_j + u_j n_i) dS \quad (14)$$

Now, it can be shown using the divergence theorem on Equation 1, together with Equations 12 and 13, that:

$$\overline{\sigma}_{ij} = \Sigma_q$$

so long as the internal boundaries are traction free. A similar procedure applied to Equation 3 will result in:

$$\bar{\sigma}_{ij} = E_{ij} + d_{ij} \quad (16)$$

where:

$$d_{ij} \equiv \frac{1}{V_{\partial V_E}} \int \frac{1}{2}(u_i n_j + u_j n_i) dS \quad (17)$$

is the kinematic contribution to internal boundaries [13, 14, 15].
For purposes of convenience, suppose that the solution to the micromechanical problem is written in the following form:

\[ \sigma_{ij}(\bar{x},t) = \Lambda_{ijkl}(\bar{x}) \Sigma_{kl}(t) \quad \text{in} \ V + \partial V \tag{18} \]

where \( \Lambda_{ijkl} \) is called the stress localization tensor, representing the unitized stress distribution obtained from various sets of boundary tractions.

Now suppose that Equation 18 is substituted into Equation 4 and this result is volume averaged (in \( V \)). The result will be:

\[ E_{ij} = C_{ijkl}^g \Sigma_{kl} + E_{ij}^l \tag{19} \]

where:

\[ C_{jmmn} = C_{ijkl} \Lambda_{kmn} \tag{20} \]

and:

\[ E_{ij}^l = \varepsilon_{ij}^l - d_{ij} \tag{21} \]

Note that the above results are somewhat different from those obtained when spatially homogeneous boundary displacements are applied \([1]\). Nevertheless, it is clear that the general structure contained in local constitutive Equation 4 is retained in global constitutive Equation 19. Note that in the global representation, the effective elastic compliance tensor, \( C_{ijkl}^g \), is not constant since the stress localization tensor \( \Lambda_{ijkl} \) depends on damage.

As a practical matter it is not convenient to evaluate Equations 20 and 21 at every point in the global analysis. Therefore, an alternative procedure may be utilized to evaluate these quantities approximately from a few analyses of representative micromechanical problems. To see how this may be accomplished, consider the case wherein the tractions shown in Figure 2 are applied to the micromechanical external boundary \( \partial V \).

For this case, Equation 2 gives:

\[ \Sigma_{11} = T_x, \Sigma_{22} = T_y, \Sigma_{33} = T_x \]
\[ \Sigma_{12} = \Sigma_{13} = \Sigma_{23} = 0 \tag{22} \]

where \( T_x \) and \( T_y \) are functions of \( t \) only. Assuming that the macroscopic response is isotropic, then it is also true that:

\[ C_{ijkl}^g = \frac{1}{3} (C_2^g - C_1^g) \delta_{ij} \delta_{kl} + \frac{1}{2} C_1^g (\delta_{ik} \delta_{jl} + \delta_{il} \delta_{jk}) \tag{23} \]
Furthermore, it can be shown that in the initial undeformed state:

\[ C_1 = \frac{1}{2G_f} = \frac{(1 + v_0)}{E_f} \]

\[ C_2 = \frac{1}{3K_f} = \frac{(1 - 2v_0)}{E_f} \]

where \( E_0 \), \( K_0 \), and \( G_0 \) are the initial macroscopic Young’s, bulk, and shear moduli, respectively, and \( v_0 \) is the initial macroscopic Poisson’s ratio.

Although we are aware that the damage does induce macroscopic anisotropy, for a first approximation we assume that it does not. The application of boundary conditions (Equation 22) will cause macroscopic constitutive equations (Equation 19) to take the following form:

\[ E_{11} - E_{11} = E_{33} - E_{33} = \frac{1}{E_g} \left[ (1 - v_g) T_x - v_g T_y \right] \]

\[ E_{22} - E_{22} = \frac{1}{E_g} \left[ T_y - 2v_g T_x \right] \]
where $E^G$ and $v^G$ are the instantaneous values of the two damage dependent macroscopic elastic moduli. Solving these two equations for $E^G$ and $v^G$ results in:

$$v^G = \frac{(E_{22} - E_2 l_1) T_x - (E_{11} - E_1 l_1) T_y}{(E_{22} - E_2 l_2)(T_x + T_y) - 2(E_{11} - E_1 l_1) T_x}$$

$$E^G = \frac{(T_y - 2v^G T_x)}{(E_{22} - E_2 l_2)}$$

(26)

It can be seen that for a given set of externally applied tractions, the solution of the micromechanics problem allows one to determine all of the quantities on the right-hand side of Equation 26 as functions of time. Thus, $E^G$ and $v^G$ can be calculated for a prescribed load history. For the case wherein the damage is not statistically isotropic, the macroscopic moduli will be anisotropic, thus requiring some generalization of the above equations.

Since it is inconvenient to perform this recursively at every point in the macroscopic problem, an alternative approximate procedure is proposed here. To see this, first note that the elastic moduli can be seen to be functions of the quotient of the applied loads and the damage tensor. Assuming that this dependence is isotropic, the relation may be written as follows:

$$E^G = E^G(D_1, D_2)$$

$$v^G = v^G(D_1, D_2)$$

(27)

where $D_1$ is the first stress invariant of the damage tensor, $d_{ij}$; $D_2$ is the second deviatoric invariant of the damage tensor; and it is assumed that the macroscopic moduli do not depend on the third deviatoric damage invariant. Thus, for example, for the case of isotropic damage:

$$d_{ij} = \frac{D_1}{3} \delta_{ij}$$

(28)

In many materials the dependence of $E^G$ and $v^G$ on the arguments in Equation 27 is weakly nonlinear, or almost linear, as long as the damage is statistically spatially homogeneous in the micromechanics problem; i.e., crack interactions have not yet produced damage localization. Thus, a first approximation for Equation 27 is a truncated first-order Taylor series expansion given by:

$$E^G = E^G_0 - E^G_1 D_1 - E^G_2 D_2$$

$$v^G = v^G_0 + v^G_1 D_1 + v^G_2 D_2$$

(29)

where the signs have been changed in the second and third terms of Equation 29 in order to ensure that the coefficients will be nonnegative.
The solutions to various micromechanics problems can be utilized to obtain the material constants $E^0_1$, $E^0_2$, $\nu^0_1$, and $\nu^0_2$, and the accuracy of the first order approximation can be assessed for the given load histories.

Although the parameters $D_1$ and $D_2$ can be evaluated so long as the micromechanics problem has been solved at every point in the global body, this will not be the case for the macromechanical problem using this alternate procedure. Therefore, it will also be necessary to develop internal variable evolution laws for $D_1$ and $D_2$. These will, in general, be of the same form as that described by the microscopic evolution laws (Equations 5 and 6), except that they will be written in terms of macroscopic state variables, i.e.:

$$\dot{D}_1 = F(E_{ij}, E'_{ij}, \bar{\alpha}^{\mu}_{ij}, D_1, D_2) \tag{30}$$

$$\dot{D}_2 = G(E_{ij}, E'_{ij}, \bar{\alpha}^{\mu}_{ij}, D_1, D_2)$$

When the ratio of the overbearing pressure to the lateral pressure is constant in time, evolution laws (Equation 30) may be integrated in time to give the following algebraic equations:

$$D_1 = F^l(E_{ij}, E'_{ij}, \bar{\alpha}^{\mu}_{ij}, D_1, D_2) \tag{31}$$

$$D_2 = G^l(E_{ij}, E'_{ij}, \bar{\alpha}^{\mu}_{ij}, D_1, D_2)$$

The choice of which form to utilize will be a pragmatic one based on the desired level of accuracy of the model. This will complete the homogenization process so that the macromechanical problem can subsequently be solved.

**Formulation of the Macromechanical Problem**

The macromechanical field equations are as follows:

1. **Equilibrium Equations:**

   $$\Sigma_{i,j} = 0 \text{ in } V_G \tag{32}$$

   $$T_i = \Sigma_{ij} n_j \text{ on } \partial V_G \tag{33}$$

   where $\Sigma_{ij}$ is the symmetric macroscopic stress tensor.

2. **Strain-displacement Relations:**

   $$E_{ij} = \frac{1}{2} \left( \bar{u}_{i,j} + \bar{u}_{j,i} \right) \tag{34}$$
(3) Constitutive Behavior:

\[ E_{ij} = C_{ijkl}^0 \Sigma_{kl} + E^i_{ij} \]  \hspace{1cm} (35)

where \( C_{ijkl}^0 \) is the damage dependent elastic compliance tensor, described by Equations 23, 24, and 26 through 29. Here \( j \) denotes differentiation with respect to the global coordinates \( x^j \). Furthermore, \( E^i_{ij} \), the macroscopic inelastic strain tensor, is given by Equation 21, with evolution laws Equations 5, 6, and 30 or 31. The above field equations are cast with boundary conditions that result in a well-posed boundary value problem that can be solved with a finite element code that is similar to that used to obtain the micromechanics solution described above.

**Example Solutions for the Micromechanics Problem**

Several example micromechanics problems have been solved by the authors for a medium that is representative of rock salt. These examples are intended to demonstrate the ability of the computational algorithm to predict the evolution of damage in heterogeneous media. The geometry in all examples is described in two dimensions by a square that is 0.1 meter on each side, as shown in Figure 3. The boundary conditions and grain structure are as shown in Figure 3, where the internal lines in the schematic diagram represent grain boundaries that are modeled as cohesive zones.

The discretized finite element mesh of the representative volume is shown in Figure 4. Note that there are a total of 55 grains, 656 nodes, and 384 elements in the area, with between 1 and 28 four-node, quadrilateral elements in each grain. Since cohesive zone elements are employed along each grain boundary, multiple nodes are required at these interfaces. This results in a total of 1,293 degrees of freedom for the example micromechanics problem, which required approximately 90 minutes of computation time.

The constitutive behavior of the crystalline grains is simulated by the Munson-Dawson viscoplastic constitutive model [3] with a Mises flow potential. Thus, the body will undergo creep under constant boundary tractions. Material parameters for both the Munson-Dawson model and the cohesive zone model are given in Table 1.

In the first example, compressive surface tractions are applied under plane stress conditions with a constant out-of-plane stress of 0.0 MPa. The vertical traction is 25.5 MPa, and the horizontal traction is 0.5 MPa. The time-dependent deformation of the salt is simulated for 1 day. Figure 5 shows the normal displacement across the cohesive zones at 1 minute. As illustrated in this figure, open cohesive zones are oriented preferentially parallel with the maximum compressive stress axis. Figures 6 and 7 show the values of \( \lambda \), defined by Equation 10, at times \( t = 1 \) hour and \( t = 1 \) day, respectively. By referring to the mesh shown in Figure 3, the evolution of the damage along the grain boundaries is evident from these figures. Damage is dominated by shear failure rather than opening mode cracking.

A second example calculation has been made by applying boundary tractions of 30.5 MPa vertically and 0.5 MPa horizontally, thus resulting in a slightly higher deviatoric stress in the body.
Figure 3. Geomechanical model of rock salt with cohesive zones.
Figure 4. Finite element mesh of rock salt model with cohesive zones.
Figure 5. Contours of relative normal displacement across the cohesive zone at 1 minute ($T_y = 25.5$ MPa; $T_x = 0.5$ MPa).
Figure 6. Values of $\lambda$ at 1 hour ($T_y = 25.5$ MPa; $T_x = 0.5$ MPa).
Figure 7. Values of $\lambda$ at 1 day ($T_y = 25.5$ MPa; $T_x = 0.5$ MPa).
Table 1. Munson-Dawson and Cohesive Zone Model Parameters

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Results for the cohesive zone displacements at time \( t = 1 \) minute, 1 hour, and 1 day are shown in Figures 8, 9, and 10. It can be seen by comparison to Figures 4 through 6 that increasing the deviatoric stress leads to accelerated damage evolution. This effect is believed to be caused by the development of shear dominated grain boundary sliding that causes subsequent crack opening and dilation in adjacent grains. Further optical observation will need to be made to determine the validity of this result.

The above example problems are intended to demonstrate the validity of the approach developed herein for predicting the response of the micromechanics problem. These results can then be applied to the homogenization principles developed above to construct the macroscopic constitutive equations required to solve the global boundary value problem.
Figure 8. Contours of relative normal displacement across the cohesive zones at 1 minute ($T_y = 30.5$ MPa; $T_z = 0.5$ MPa).
Figure 9. Values of $\lambda$ at 1 hour ($T_y = 30.5$ MPa; $T_x = 0.5$ MPa).

- $0.1 < \lambda < 0.2$
- $0.2 < \lambda < 0.3$
- $\lambda_{\text{max}} = 0.29$
Figure 10. Values of $\lambda$ at 1 day ($T_y = 30.5$ MPa; $T_x = 0.5$ MPa).
Conclusion

The authors have developed a computational model for predicting the response of microscopically heterogeneous media that undergo damage evolution. While this technique is complicated, it appears to be both efficient within current computer capabilities. However, actual comparisons of model predictions to experimental results should be carried out before quantitative assessments can be made. The authors are proceeding with these comparisons at this time.

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