PAPER NUMBER: USA-411

SAND98-0466C
SAND--98-0466C
CONF-980620--

Micromechanics and Homogenization Techniques for Analyzing the Continuum Damage of Rock Salt

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ABSTRACT

This paper presents a model for evaluating microcrack development and dilatant behavior of crystalline rocks. 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. The model is capable of describing the evolution from initial debonding through complete separation and subsequent void growth of an interface. An example problem of a rock salt specimen subjected to a high deviatoric load and low confinement is presented that predicts preferential opening of fractures oriented parallel with the maximum compressive stress axis.

KEYWORDS

Constitutive modeling, dilation, micromechanics, salt, damage, microcracks

INTRODUCTION

Most geomechanical evaluations of underground structures in rock salt assume that the salt is homogeneous. This approximation is sufficiently accurate if the geometric scale of the heterogeneities is small compared to the size of the structure modeled. However, rock salt can demonstrate a significant amount of heterogeneity when viewed on a scale at which individual grains are observed. In particular, the formation of microcracks can induce a significant amount of heterogeneity that changes the characteristic behavior of salt. The interaction of the inelastic deformation and microcracking determines the macroscopic behavior of the salt matrix. The transition from steady-state creep to tertiary creep is an example of this interaction.

The actual formation of cracks in salt during deformation is very difficult to observe. Nevertheless, it seems worthwhile to consider the form that new cracks might have and the ways in which they might originate.

DISCLAIMER

Three possible types of cracks are shown in Figure 1 for an axisymmetric specimen subject to an axial load σ_a and confining pressure σ_c. The simplest possibility is the isolated axial crack (Figure 1a). The axis of this crack is oriented parallel with the maximum compressive stress axis. Open axial cracks might also form at the junctions of three grain boundaries or three preexisting cracks, two of which are inclined and one is axial (Figure 1b). Sliding along the two inclined surfaces is accommodated by opening of the axial crack. The third possibility (Figure 1c), which is related to the second, is that axial cracks might form at either end of a preexisting crack or grain boundary that is inclined to the principal stress axis. Again, sliding along the inclined surface can be accompanied by opening of the crack at either end of the inclined surface.

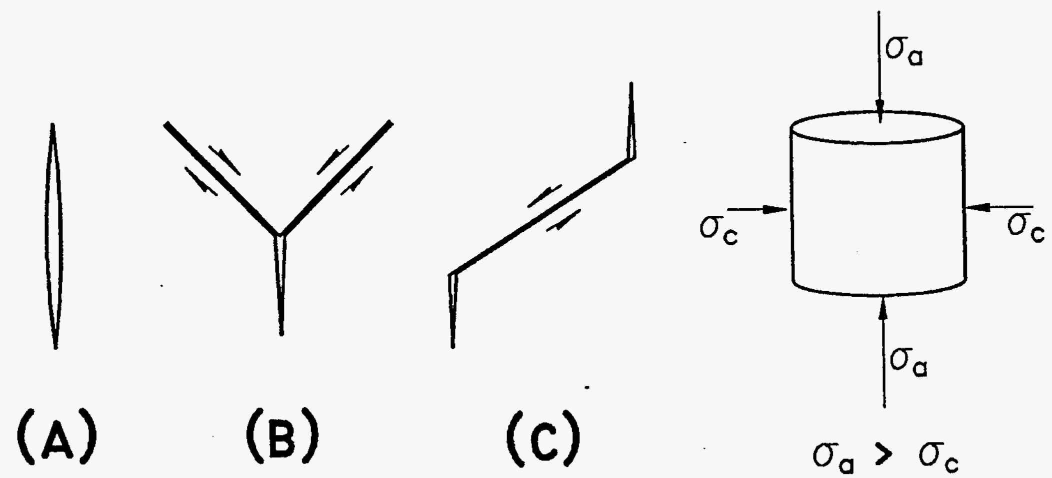

Figure 1: Three possible types of open cracks along or at grain boundaries

In this paper, a modeling approach is presented for predicting the creep and damage evolution (i.e., inelastic deformation resulting from the creation of new microcracks or opening of existing microcracks) in rock salt at the grain scale. It is postulated that microcrack formation is dominated by grain boundary sliding and opening. Therefore, if an appropriate model can be determined for predicting the interface behavior between salt grains, a micromechanics problem can be formulated and solved by the finite element method. Currently, the deformation mechanisms of interest are limited to intragranular creep and intergranular sliding and dilation of grain boundaries.

MODELING APPROACH

There are two fundamentally different approaches to obtain macroscopic constitutive equations for predicting damage (Boyd *et al*, 1993): (1) a micromechanics approach and (2) a phenomenological approach. The phenomenological approach assumes that all the information can be obtained from experiments performed on test specimens whose dimensions are large compared to the asperities. For rock salt, asperities could include impurities contained within the salt matrix, or preexisting or newly formed microcracks. The information obtained from the experiments is used to determine parameter estimates for an assumed constitutive model to predict the macroscopic behavior of the material.

The micromechanics approach assumes a constitutive behavior for each component material contained within the test specimen. Typically, the behavior of the component materials is described by less complex constitutive models than the composite material because component models are usually isotropic. A micromechanics analysis of a representative volume element of the composite material can account for the heterogeneity caused by spatial variation of materials and cracks. Macroscopically averaged constitutive equations can be obtained by averaging the results of a micromechanics problem for a representative volume. This process of averaging the micromechanics solution to obtain the locally averaged constitutive equations is often termed homogenization. When a homogenization procedure (e.g., Costanzo *et al*, 1996) is applied to the micromechanics solution, the resulting macroscopic equations should, in principle, be equivalent to that which would be obtained by the phenomenological approach. However, the micromechanics approach has the added benefit of providing additional information regarding local phenomena (e.g., microcrack density, aperture, orientation, and tortuosity) that are not necessarily determined by the phenomenological approach.

Micromechanics and homogenization methods have been utilized to develop constitutive models for crystalline rock (e.g., Ichikawa *et al*, 1996; Handley, 1996). The micromechanics approach begins with the formulation of a heterogeneous micromechanics problem. For granular aggregates, such as rock salt, it is postulated that stress concentrations at grain contacts enhance the probability of fracturing. The orientation of the grain boundaries with respect to the principal stress axes determines where fractures initiate. After fracture occurs in either the grain with the greatest stress concentration or the grain possessing a critical flaw, the load is distributed to neighboring grains; thus, promoting a continuation of fracturing. Therefore, a micromechanics analysis of damage development in salt requires, at a minimum, that individual salt grains and the interaction between salt grains be modeled.

MICROMECHANICS MODEL

The deformation of salt can be decomposed into thermal expansion, elastic deformation, and inelastic deformation. The inelastic deformation is highly stress-, temperature-, and rate-dependent. It includes both viscoplastic and brittle components with the viscoplastic component usually dominating in the range of stress and temperature expected in the salt surrounding underground workings in rock salt. The dislocation processes are assumed to be pressure-insensitive and incompressible for rock salt. The dislocation mechanisms defined by the Munson-Dawson (M-D) model (Munson *et al*, 1989) are used here to model the isovolumetric behavior of individual salt grains. The framework for the damage model reported herein is based on the assumption that microcracks form exclusively at grain boundaries. Therefore, it is assumed that the dilatant behavior of rock salt can be predicted by a model that simulates microcracking at preexisting locations within the salt matrix. Microcracking and dilation at grain boundaries are modeled here by employing a cohesive zone model. The cohesive zone model proposed by Tvergaard (1990), and similar to that developed by Needleman (1987), is used here with minor modifications.

The cohesive zone model is a formulation for an interface that accounts for separation via nonlinear constitutive behavior. The mechanical behavior of this model is described through a constitutive relation that gives the dependence of tractions along the interface surface on both relative normal and shear displacement across the interface. The special behavior of this model may relieve the stress and/or strain singularity that otherwise would be predicted at the crack tip of a sharp crack. The model is capable of describing the evolution from initial debonding through complete separation and subsequent void growth at an interface. The disadvantage to this modeling approach is that the grains can never fail, and the rupture paths are predefined (i.e., by the positions of the grain boundaries).

Cohesive Zone Model

Cohesive zone models have been used by several researchers (e.g., Tvergaard and Hutchinson, 1993; Allen *et al*, 1995; Lo and Allen, 1994) to successfully model the evolution of damage in metals and metal-matrix composites. The cohesive zone model utilizes a traction-displacement relationship to produce a smooth transition from displacement continuity along predetermined internal surfaces to traction-free internal boundaries. The constitutive equations for the interface are such that with increasing interfacial separation, the tractions across the interface reach a maximum and then decrease and eventually vanish so that complete debonding occurs. The model is a phenomenological continuum-level depiction of the relation between interatomic bond forces and interatomic bond separation. This relationship is depicted in the nondimensional graph for purely normal separation shown in Figure 2. In Figure 2, T_n is the normal traction, σ_{max} is normal bond strength, u_n is normal separation, and δ_n is the interface failure separation.

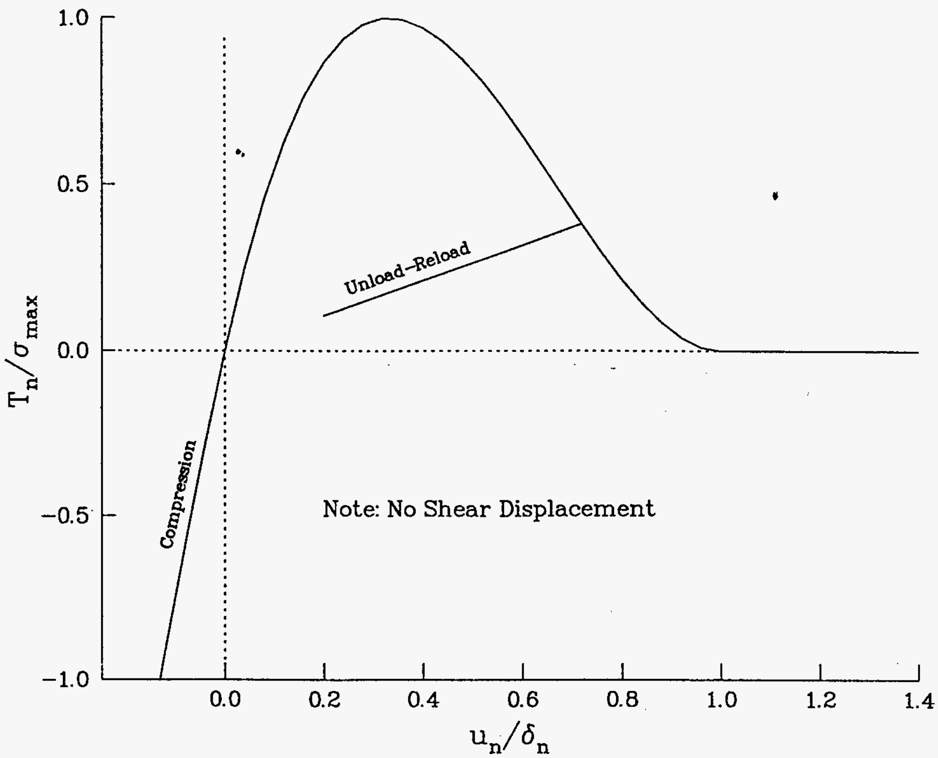

Figure 2: Normal interface tractions versus interface separation for the cohesive zone model

The current cohesive zone model follows the work of Tvergaard (1990) who did not derive expressions for the tractions through a potential. Tractions are defined based on both the relative normal (u_n) and shear (u_s) displacements and the bond strength. In two dimensions, the normal (T_n) and shear (T_s) tractions along a cohesive zone interface are defined as:

$$T_n = \left(\frac{27}{4}\right)\sigma_{max}\left(\frac{u_n}{\delta_n}\right)(1-\lambda)^2 \qquad 0<\lambda<1 \tag{1}$$

$$T_s = \alpha\left(\frac{27}{4}\right)\sigma_{max}\left(\frac{u_s}{\delta_s}\right)(1-\lambda)^2 \qquad 0<\lambda<1 \tag{2}$$

where:

$$\lambda = \sqrt{\left(\frac{u_n}{\delta_n}\right)^2 + \left(\frac{u_s}{\delta_s}\right)^2} \tag{3}$$

and δ_n and δ_s are length scales associated with debonding and α is a material property relating shear to normal strength. It can be seen from Eqns. 1 through 3 that the normal and shear tractions are coupled to the normal and shear displacements. Considering purely normal separation, the maximum normal traction is reached when $\lambda = 1/3$. The maximum normal traction is equal to the bond strength (σ_{max}) as illustrated in Figure 2. If the cohesive zone is loaded beyond $\lambda = 1/3$, the imposed traction decreases with increasing displacement until $\lambda = 1$. For values of $\lambda \geq 1$, the cohesive zone is fully debonded.

If the cohesive zone is loaded beyond $\lambda = 1/3$ and unloaded, Eqn. 1 will yield an increasing traction for a decreasing displacement. Because this is not physically reasonable, the model was modified to provide a better representation of the postpeak unloading response. Following the work of Foulk (1997), a linear unload/reload traction-displacement relationship is assumed as illustrated in Figure 2. This is accomplished by replacing λ in Eqns. 1 and 2 with λ_{max}, where λ_{max} is the maximum value of λ before unloading. These relationships are used when $\lambda_{max} \geq 1/3$ and $\lambda \leq \lambda_{max}$.

One other modification was made to the model introduced by Tvergaard (1990) to describe the force behavior when the cohesive zone element is loaded in compression. Under compressive loading conditions, the relative normal displacement of the cohesive zone is negative ($u_n < 0$). A nonlinear traction-displacement relationship is predicted by Eqn. 1 in compression. Depending on the loading condition and modeled geometry, this relationship may not be suitable for limiting the penetration across the cohesive zone. Additionally, the normal traction given by Eqn. 1 is a function of the shear displacement and decreases after λ exceeds 1/3. To circumvent this problem, a nonlinear relationship was developed when normal penetrations exist ($u_n < 0$) as follows:

$$T_n = \left(\frac{27}{4}\right)\sigma_{max}\left(\frac{u_n}{\delta_n} + (\beta - 1)\left(\frac{1-\cosh\left(\frac{u_n}{\delta_n}\right)}{\sinh(1)}\right)\right) \tag{4}$$

$$T_s = \alpha\left(\frac{27}{4}\right)\sigma_{max}\left(\frac{u_s}{\delta_s}\right)\left(1 - \frac{|u_s|}{\delta_s}\right)^2 \tag{5}$$

where β is a constant of magnitude sufficient to limit interpenetration. Note that the normal traction is not coupled to shear displacement in Eqn. 4. Similarly, the shear traction is not coupled to normal displacement across the cohesive zone (see Eqn. 5). Figure 2 illustrates the normalized traction-displacement relationship in compression ($u_n/\delta_n < 0$) using Eqn. 4. The imposed traction is monotonically decreasing based on the relative displacement. This results in a continuous material stiffness for purely normal displacement. The functional form implemented to limit penetration becomes highly nonlinear for large values of β, which makes convergence more difficult and increases computation time.

EXAMPLE PROBLEM RESULTS

As previously discussed, the volume average of a micromechanical analysis should be the same as that obtained by macroscopic constitutive equations, with minor discontinuities, at a size greater than or equal to a representative volume element (RVE). An RVE may be defined for rock salt as the size beyond which very little variation is found in the macroscopically averaged mechanical or hydrological properties of the rock mass. 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 of the example problems (which is not intended to be a representative volume element) is described in two dimensions by a square that is 0.1 meter on each side. 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. Each of the polygons in Figure 3 is characterized by the M-D model; thus, the body will undergo creep under time-independent boundary tractions. Material parameters for both the M-D model and the cohesive zone model are given in Table 1.

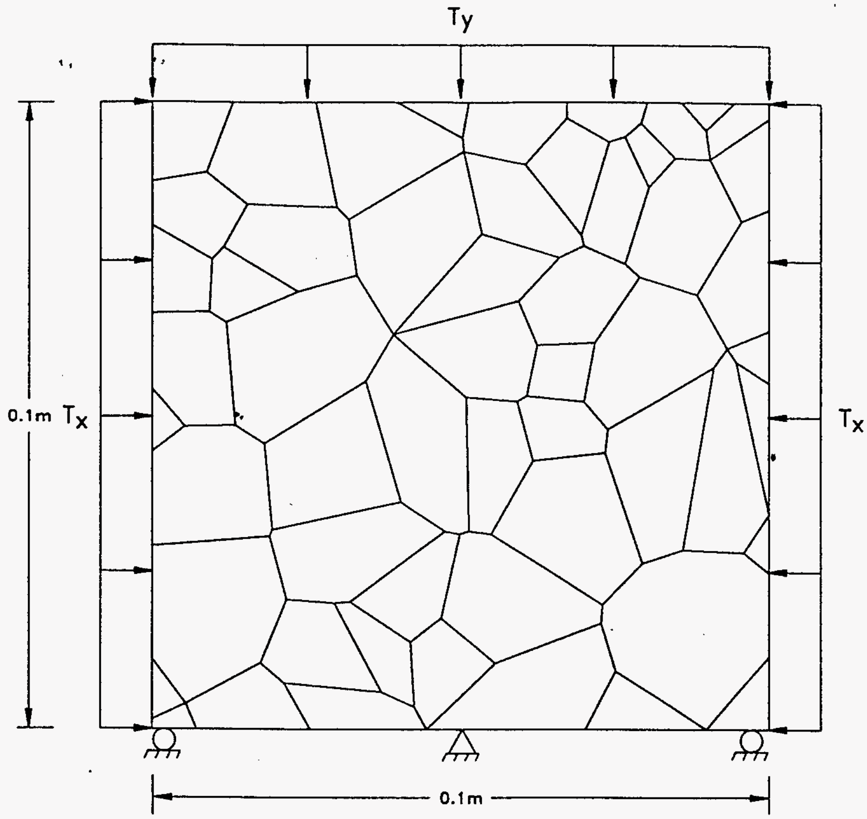

Figure 3: Voronoi polygon granular model (after Handley, 1996)

The finite element mesh of the 55 grains shown in Figure 3 is comprised of 656 nodes and 384 elements, with between 1 and 28 four-node quadrilateral elements in each grain. Because 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 was solved on a DEC Alpha 3500 computer using the finite element program **SPECTROM-32**, Version 4.10 (Callahan *et al*, 1989).

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 4 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 5 and 6 show the values of λ (Eqn. 3) at 1 hour and 1 day, respectively. The evolution of the damage along the grain boundaries is evident from these figures. The damage is dominated by shear failure rather than crack opening.

DISCUSSION AND SUMMARY

A micromechanics-based methodology has been proposed to predict damage in rock salt. A cohesive zone model was used to predict interface sliding and dilatant behavior along salt grain boundaries. The special behavior of this model may relieve the stress and/or strain singularity that otherwise would be predicted at the tip of a sharp crack. Solutions to example problems indicate that the approach is capable of predicting a dilatant response through propagation and coalescence of interface separations, with increasing damage predicted in accordance with an increasingly greater deviatoric stress. However, the damage is dominated by shear failure rather than crack opening if subject to a constant load. Microscopy studies clearly identify that the primary change in microstructure associated with creep-induced damage is grain boundary dilation. Therefore, it appears that model modification is required to accurately predict damage accumulation in rock salt. Due to the nature of the cohesive zone model employed, the critical energy criterion that must be overcome for crack extension to occur is a constant. This is not always the case in inelastic media and may well be an oversimpification in salt.

TABLE 1
M-D AND COHESIVE ZONE MODEL PARAMETER VALUES

Parameter	Units	Value
Elastic Parameter Values		
E	MPa	31,000
ν	—	0.25
μ	MPa	12,400
M-D Creep Parameter Values		
A_1	s^{-1}	8.386×10^{22}
A_2	s^{-1}	9.672×10^{12}
Q_1	cal/mol	25,000
Q_2	cal/mol	10,000
n_1	—	5.5
n_2	—	5.0
B_1	s^{-1}	6.0856×10^{6}
B_2	s^{-1}	3.034×10^{-2}
q	—	5,335
σ_o	MPa	20.57
m	—	3.0
K_o	—	6.275×10^{5}
c	K^{-1}	9.198×10^{-3}
α	—	−17.37
β	—	−7.738
δ	—	0.58
Cohesive Zone Parameter Values		
δ_n	m	1.75×10^{-4}
δ_s	m	1.75×10^{4}
σ_{max}	MPa	10
α	—	1.5
β	—	1.0×10^{6}

While this methodology may be complicated, there are numerous advantages of using the micromechanics approach over the phenomenological approach (Suquet, 1986; Boyd *et al*, 1993). One advantage of using the micromechanics approach is that only the behavior of the constituents, which may be isotropic, needs to be evaluated, even though the macroscopic behavior may be anisotropic. Another advantage is that the micromechanics solution will give macroscopic properties that apply for any mixture of volume fraction of constituents. Additionally, a micromechanics analysis of a representative volume element could provide information regarding the microstructure including fracture density, aperture, and tortuosity of microfractures in salt subject to different loading conditions. This information could provide valuable insight for characterizing the disturbed rock zone around underground openings in rock salt.

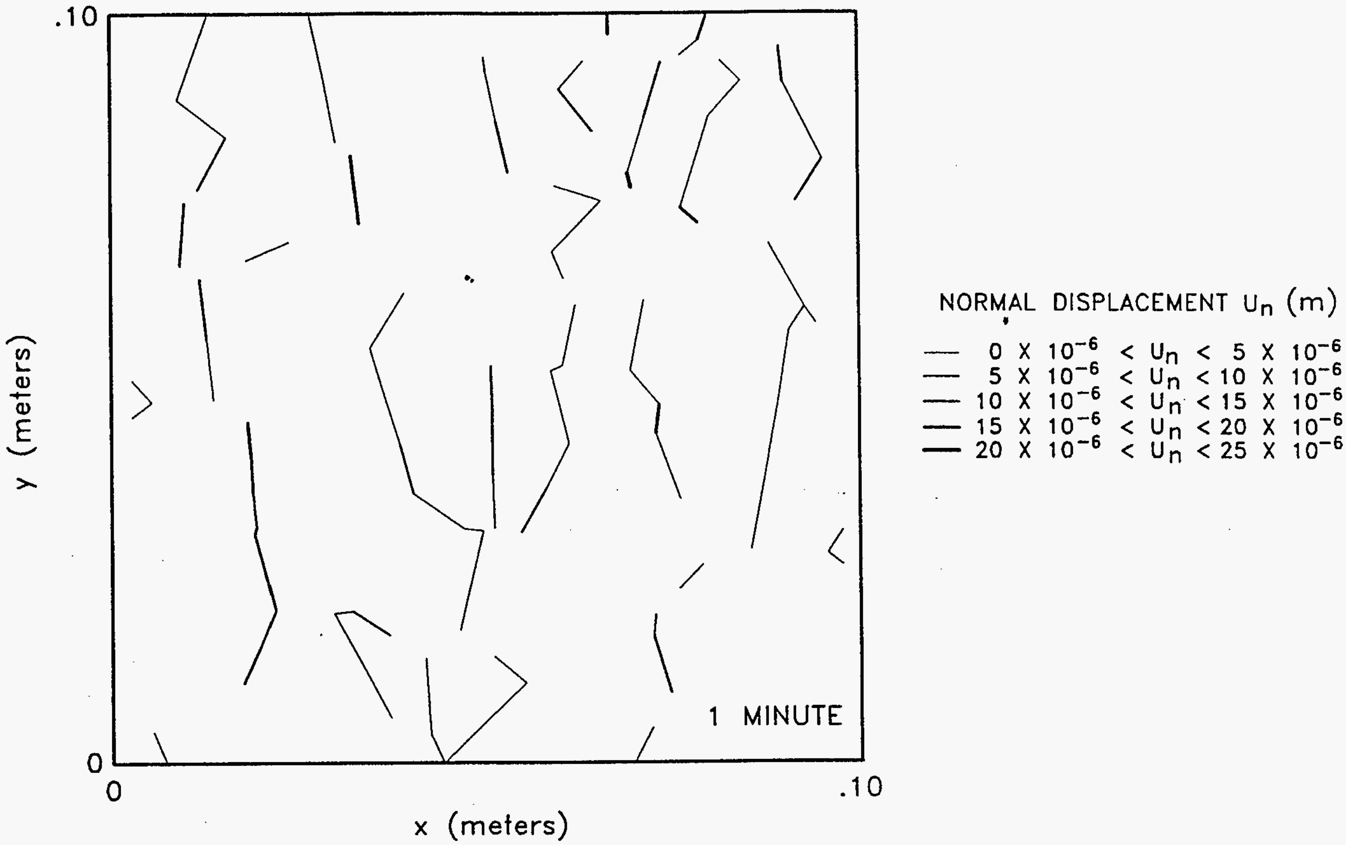

Figure 4: Contours of relative normal displacement across the cohesive zones at 1 minute (T_y = 25.5 MPa; T_x = 0.5 MPa)

For purposes of analyzing large-scale problems, it is untenable to model each grain boundary with a cohesive zone. Assuming the model of the micromechanics problem represents a periodic structure of salt at the microscale, the solution to this problem can be homogenized to produce a macroscopically homogeneous constitutive model that can be utilized in large-scale analyses. This is accomplished by volume averaging the solution to the micromechanics problem utilizing homogenization principles. The resulting constitutive equations can be implemented into a finite element program to provide an efficient method of modeling the evolution of damage in rock salt. The load history determined at discrete points in the macroscale analysis can then be applied to the micromechanics problem to analyze the material behavior at the grain scale.

ACKNOWLEDGMENTS

Work for this study was conducted through Sandia National Laboratories. Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy under Contract DE-AC04-94AL85000.

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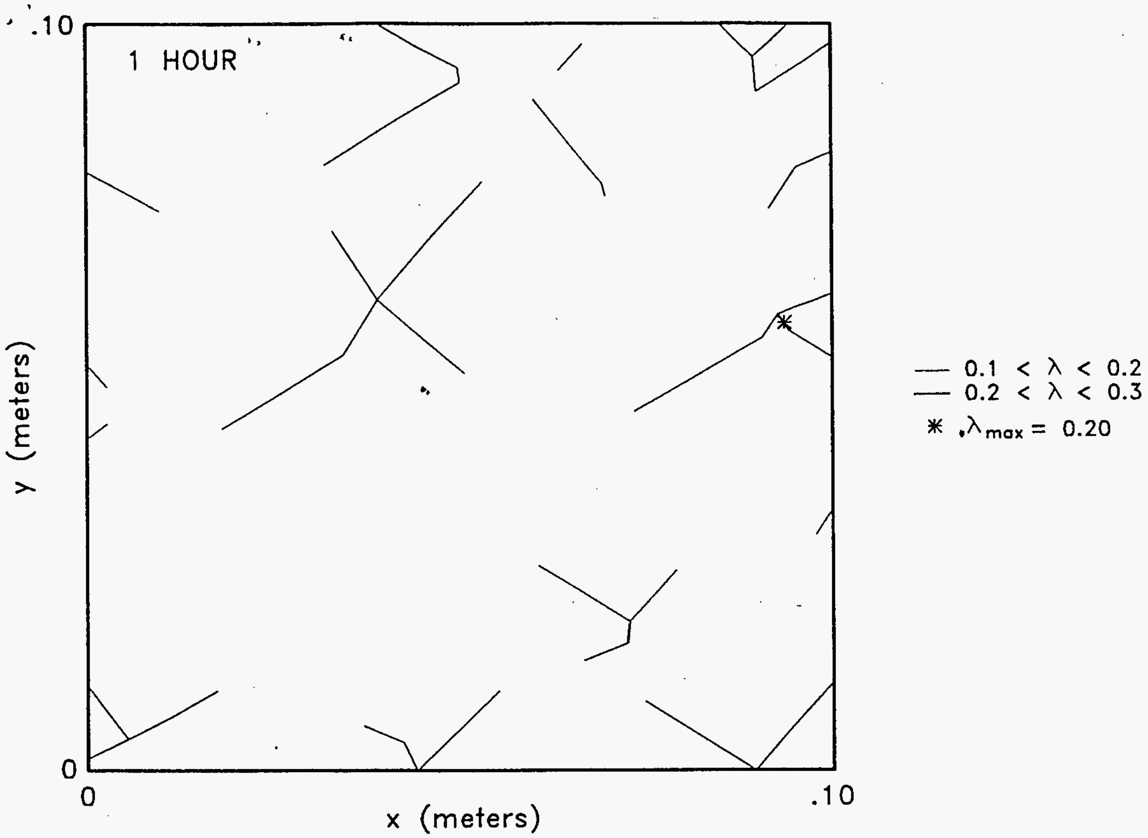

Figure 5: Values of λ at 1 hour (T_y = 25.5 MPa; T_x = 0.5 MPa)

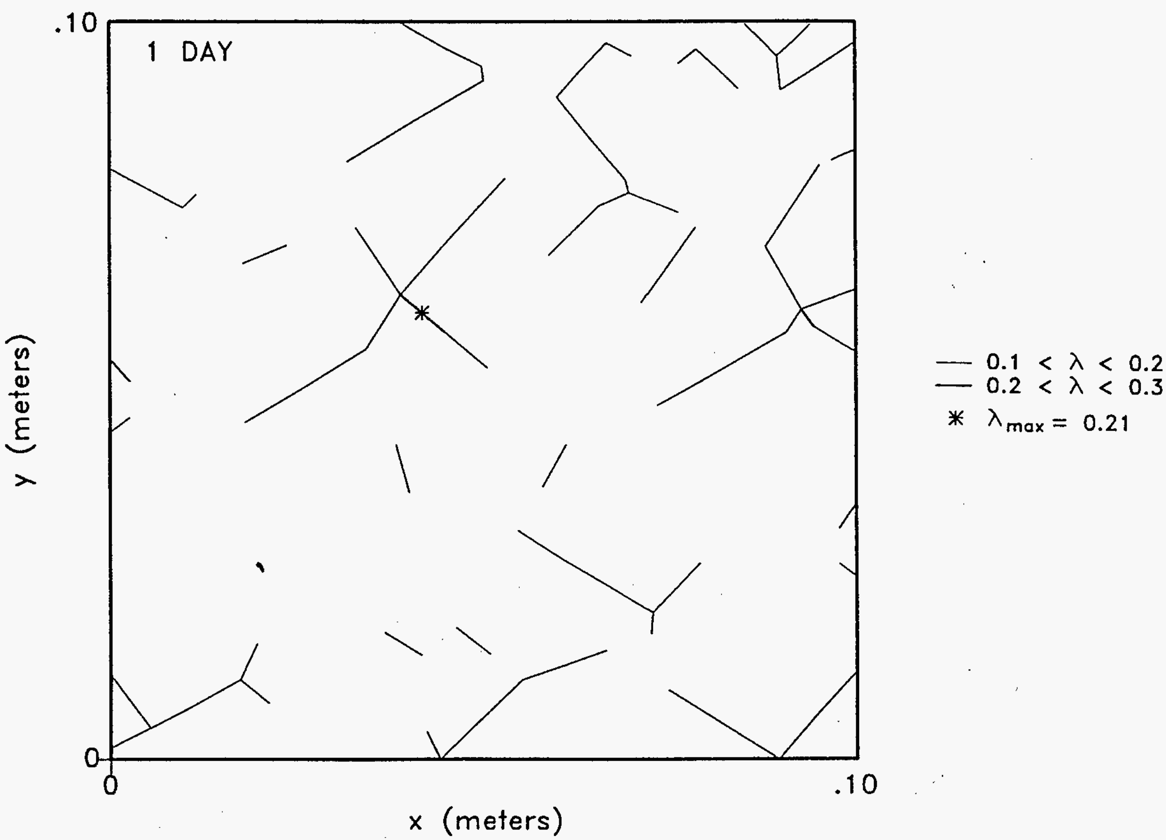

Figure 6: Values of λ at 1 day (T_y = 25.5 MPa; T_x = 0.5 MPa)

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M98004243

Report Number (14) SAND--98-0466C

CONF-980620--

Publ. Date (11) 199803

Sponsor Code (18) DOE/EM, XF

UC Category (19) UC-2000, DOE/ER

DOE