Preliminary Submission: Numerical Modeling of Granular Salt

Brandon Lampe and Laxmi Paneru

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Nomenclature

 $\dot{\epsilon} = \text{Strain rate}$

 $Q_a = Activation energy$

R =Universal gas constant

T = Absolute temperature

 $C_1 = \text{Constant factor}$

1 Introduction

Granular (or crushed) salt is a candidate material for sealing the Waste Isolation Pilot Plant's (WIPP) shafts, drifts, and boreholes; therefore, the ability of crushed salt to prevent fluid migration is of interest. The objective of our research is to better understand the mechanical properties of crushed salt as they pertain to its transport properties, most notably its intrinsic permeability, which will provide a direct measure of its adequacy as a sealing material. Because a materials permeability is directly related to the pore volume of the material (along with connectivity of the pores), we are currently focusing on the ability of a constitutive model to accurately predict volumetric strain. In a effort to complete this objective, we have performed a suite of laboratory tests on crushed salt over a variety of conditions and have measured it's transient deformation.

The following sections will first familiarize the reader with existing constitutive models. Then a description of typical test methods and results are presented. A brief description of the currently employed constitutive models is provided followed by the model description and results. We will compare the results of different constitutive models to our measured data and quantify the ability of these models to predict the measured strain values.

2 Literature Review

Mechanical properties of in situ salt were first well characterized by Munson and Dawson during the early 1970's[7], where they first utilized an Arrhenius type equation to describe the time dependent

deformation of salt, which is now common practice, this relationship is shown below:

$$\dot{\epsilon} = C_1 * exp\left(\frac{-Q_a}{RT}\right)$$

During that same period, crushed salt became of interest to the engineering community also, predominately for use as a seal material around nuclear wast packages, shafts, and other openings associated with the storage of nuclear waste. The first recorded laboratory tests, performed for obtaining constitutive parameters were uniaxial compression tests completed in 1978 on samples that were 5 centimeters in diameter [6]. However, the small specimen sizes utilized in these early tests had nonuniform stress fields (from side and end friction) producing inconsistent results. Since the first tests on crushed salt were performed, testing techniques have advanced greatly and we are now able to accurately measures strains at at high temperatures and pressures that are representative of downhole conditions in a nuclear waste storage facility[2].

During the last 39 years, over ten constitutive models have been developed for crushed salt, each based on varying degrees of phenomenology, micro mechanics, and/or empiricism[4]. During the mid-1990's, the Crushed Salt (CS) model was developed, with funding from the US Dept. of Energy, which was the first model to combine several dominant deformation attributes of crushed salt, such as grain boundary pressure solutioning and dislocation creep, which are believed to be dominant deformation mechanisms of crushed salt [9, 10, 3]. Including these different deformation mechanisms is critical to accurately predicting the deformation of salt, as the dominant mechanism varies with local conditions [5]. The CS model has the ability to predict the deformation of crushed salt reasonably well at low temperatures, but at high temperatures Broome et al. [2] showed the model predictions did not well represent the true deformations. An additional shortcoming of the CS model is the large number of material parameters (constants) associated with it, 31 independent parameters in total, which produce a highly nonlinear result that makes fitting parameters to a specific salt deposit very difficult. The US Dept. of Energy currently utilizes the CS model to aid in there planning and development of storage facilities; therefore this model is of particular interest to us.

More recently, Olivella and Gens [8] developed an additional constitutive model that utilizes a nonlinear viscous approach that again focused on capturing the deformation associated with the active deformation mechanisms at different conditions. This model is currently employed by the THERESA project, which is a European based group aimed at developing, verifying and improving the modeling capabilities associated with the storage of nuclear waste. We do not currently have access to this model; therefore, this model will not be analyzed at this time.

3 Test Methods and Results

The laboratory data was obtained during a hydrostatic and shear compression tests of a crushed salt, approximate specimen geometry is shown in Figure 1. Axial displacements were measured via linear variable differential transformers (LVDTs) placed external to the specimen, lateral displacements were measured with a pair of Shuler gages placed circumferentially around the specimen, and metering of the confining fluid volume. Results from the measured strains are shown in Figure 2 along with the resulting reduction in porosity shown in Figure 3.

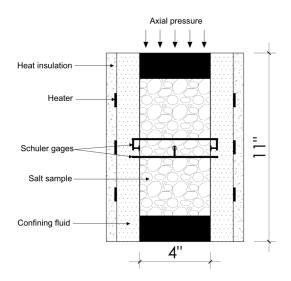


Figure 1: Representation of crushed-salt specimen in the triaxial cell.

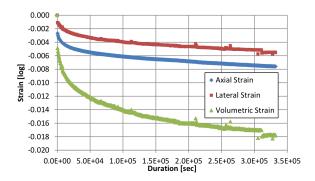


Figure 2: Strain measures during the hydrostatic compression test.

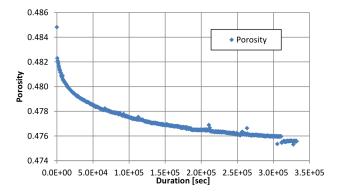


Figure 3: Calculated porosity during a hydrostatic compression test.

4 Constitutive Models

We plan to predict the deformation measured during laboratory tests using the following constitutive models:

- Generalized Hooke's law for linear elasticity
- Drucker-Prager/cap plasticity
- CS Model

The first two constitutive models may be implemented using Abaqus once the material parameters are obtained from tests data[1]. However, Abaqus does not contain the CS model in its library, but we wish to compare results of the CS model to other existing models. Therefore, we have programmed the CS model in the R language, and our algorithm produces the predicted strains from the CS model. This implementation of the CS model allows for the comparisons with other constitutive models in the Abaqus library when a single element is utilized.

5 Model Description

Numerical analyses were performed using the program Abaqus/CAE 6.14-1 to perform the finite element analyses. Abaqus contains a range of constitutive models and elements to choose from. Currently, our finite element model contains 1,566 nodes and 1170 8-node brick elements. We plan on complete multiple meshes of our model with both less and more elements to determine how many elements are needed for convergence of a solution.

Our model geometry consists of two end platens modeled as linear elastic aluminum and the test specimen, which is (*will be) be modeled as both an elastic and viscoplastic material. The test specimen was assumed to contain two orthogonal planes of symmetry, each with essential boundary conditions (zero displacement). The upper platen was also defined with an essential boundary condition of zero displacement. The lower platen and the curved face of the specimen were both defined as having natural boundary conditions (prescribed force). The boundary condition on the curved face of the specimen were defined as a constant pressure (no shear component) that represents the confining fluid. Additionally, the lower platen was prescribed an constant pressure. Magnitudes of the prescribed natural boundary conditions varied depending on the simulated test scenario (e.g., were equal for hydrostatic compression test and not equal shear compression test). Interactions between the salt specimen and the end platens were also modeled in attempt to capture the influence of end affects.

6 Numerical Results

Very limited results have been obtained thus far, below Figures 4 and 5 show the deformed mesh with contour plots of the numerical results. These results were obtained from modeling a linear elastic specimen under a hydrostatic stress of 200 pounds per square inch (psi). These initial results verified that essential boundary conditions are acting as intended, i.e. zero displacement at the upper platen and across the planes of symmetry. Natural boundary conditions also appear to be correctly implemented as the material as uniformly deformed in and up as was expected from a linear elastic model. Frictional affects between the platens and specimen also appear to be captured, as the stress distribution is not radially uniform at the specimen ends, which was expected.

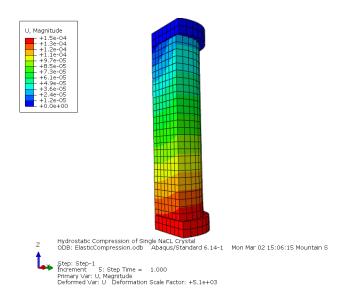


Figure 4: Numerical displacement (inch) results from a linear elastic simulation performed in Abaqus.

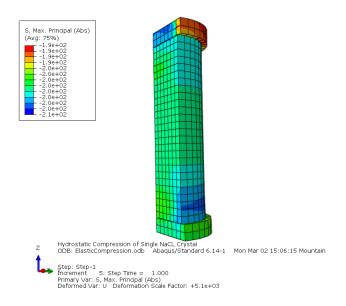


Figure 5: Numerical stress (psi) results from a linear elastic simulation performed in Abaqus.

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