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Formulation of a Constitutive Equation for Salt

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ABSTRACT

A constitutive model has been developed to simulate the time-dependent brittle–ductile behavior of salt and to overcome some basic difficulties of finite element modeling (FEM). Conventional FEM is usually inadequate for quantitative prediction of behavior of complex earth structures in general and salt openings in particular. The present model is constructed in a modular fashion based on natural laws to incorporate failure, postfailure, and long-term creep deterioration realistically to simulate long-term behavior of geologic materials. It is applicable to a wide range of earth materials, including water, soil, fractured mass, and salt by properly reflecting the numerical values of the property coefficients.

INTRODUCTION

Production of salt provides the byproduct of a large underground space which is often found to be far more valuable than the salt itself. The list of commodities being stored in salt spaces is rapidly expanding and now includes oil, gas, LPG, compressed air, chemicals, and wastes, with the possible addition of grains and LNG. The long-term stability of the salt space thus becomes important.

Creep, deterioration, and failure of salt will govern the long-term integrity of storage caverns with respect to their mechanical stability and hydrological containment. Given the likelihood of increased utilization of underground space in salt, with increasing demand for design performance, it is clear that a realistic mathematical representation of salt mechanics is needed to describe the behavior of underground space under complex *in situ* conditions.

Numerous constitutive models have been developed in an attempt to describe the mechanical behavior of salt. Most models have been specifically derived to predict long-term creep deformation and have overlooked the importance of brittle failure associated with long-term creep. Omission of the brittle behavior sometimes poses an unrealistic assumption and results in a misunderstanding of observed deformations. Therefore it is highly desirable for salt cavern analysis to use a constitutive model which incorporates the brittle–ductile duality of salt behavior. Unfortunately, this most important requirement has rarely been met.

This paper describes the mathematical formulation of a constitutive equation proven effective for design and analysis of underground spaces. The derivation of the equation is given in generalized form and its adaptation to salt is specified. The unique characteristics of the equation are discussed with reference to field applications. Field application examples are given in two other papers in this volume (Dickie et al., 1993; Mehta and Serata, 1993).

SCHEME OF CONSTITUTIVE EQUATION

Figure 1 gives the modular system of the major (primary) behavioral components comprising the constitutive equation, showing the separation of the octahedral shear stress–strain relation (τ_o–γ_o) from the mean stress–strain relation (σ_m–ε_m). These two relationships act in parallel and are closely related to each other via the failure and postfailure conditions of the stresses and strains. They are independently analyzed because they produce mutually

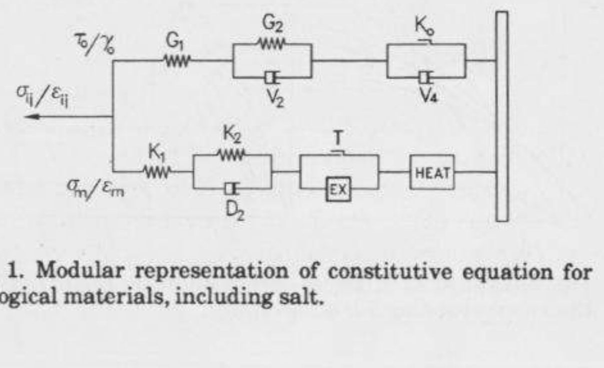

Fig. 1. Modular representation of constitutive equation for geological materials, including salt.

opposing effects: the (τ_o–γ_o) relation represents a destructive mechanism, while the (σ_m–ε_m) relation represents a strengthening mechanism. The deformation and failure of materials at a given moment is merely a balance between these effects. The model simultaneously describes the shear behavior (by a linear sum of the elastic, viscoelastic, and viscoplastic strain components) and the mean behavior (by a linear sum of the elastic, viscoelastic, volumetric expansion [dilation], and thermal expansion strains).

Tables 1 and 2 give descriptions for the primary and secondary geological property coefficients, as well as their numerical values for rock salt. These coefficients can be determined by conventional creep and strength testing (e.g., ASTM D4406) and by transition, model cavity, and penetrometer testing (i.e., Serata, 1961; Serata et al., 1986, 1991). All coefficient values for salt are determined from laboratory test results by Serata Geomechanics, Inc. (SGI) and Sandia National Laboratories. The geomechanical characterization and mathematical derivation of the constitutive equation are described below.

Failure strength

The failure strength K_o of all earth materials increases with an increase of mean stress σ_m toward the ultimate value of K_o^B. The rate of the increase is found to obey the natural law with respect to σ_m as:

$$dK_o/d\sigma_m = \alpha(K_o^B - K_o) \quad (1)$$

where: α = yield surface coefficient, and K_o^B = ultimate octahedral shear strength.

Equation (1) leads to the following expression of failure strength, which is applicable for brittle to ductile materials:

$$K_o = K_o^A + (K_o^B - K_o^A)\,[1 - \exp(-\alpha\sigma_m)] \quad (2)$$

where: K_o^A = unconfined octahedral shear strength.

Figure 2 gives typical test results of salt specimens, illustrating the axial stress–strain (σ_a–ε_a) prior to and after failure in relation to the 3-D stress state (τ_o–σ_m).

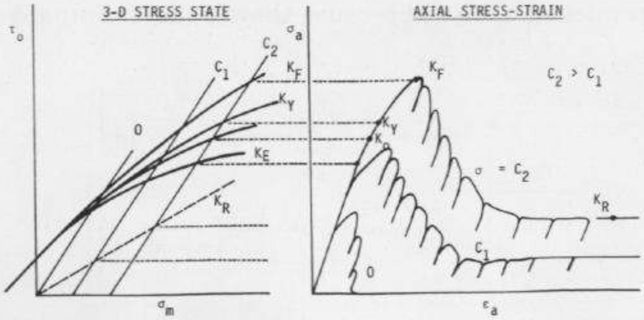

Fig. 2. Typical axial stress–strain relations compared with their corresponding 3-D stress states.

TABLE 1

Primary geological property coefficient values of rock salt

Coefficient	Definition	Dimension	Range
G_1	Shear modulus	10^9 Pa	1.4–15
G_2	Retarded shear modulus	10^9 Pa	0.7–10
V_4	Plastoviscosity	10^9 Pa day	3.5-15
K_o^A	Unconfined octahedral shear strength	10^6 Pa	0.1-1.5
K_o^B	Ultimate octahedral shear strength	10^6 Pa	4-7
V_2	Elastoviscosity coefficient	10^9 Pa day	0.7-1.5
K_1	Bulk modulus	10^9 Pa	13-28
K_2	Retarded bulk modulus	10^9 Pa	0.7-2.8
D_2	Hydrostatic elastoviscosity	10^9 Pa day	3.5-15

TABLE 2

Secondary geological property coefficient values of rock salt

Coefficient	Definition	Dimension	Range
L	Thermal coefficient of viscoplasticity	1	9.0-9.8
n	Nonlinear coefficient of shear stress effect to viscoplastic state	1	1.6-2.6
b	Nonlinear coefficient of confinement to viscoplastic state	1	2.0-2.4
α	Yield surface coefficient	1/kPa	0.21-0.23
γ_c	Critical shear strain of failure	10^{-3}	3-4
F	Failure point	1	1.8-2.2
P	Plastic point	10^6 Pa	35-40
T	Tensile strength	Pa	0-1.0
J	Shear expansion coefficient	1	0.001-0.01
H	Confinement coefficient	1	0.1-1.0
Th	Linear thermal expansion constant	1/°K	$110\text{-}130\times10^{-6}$
K_{NN}	Thermal conductivity in NN direction	W/m·K	2-10
C_p	Specific heat	J/kg·K	$10\text{-}12\times10^6$

Viscoelastic behavior

The viscoelastic (VE) state is defined as the state in which the octahedral shear stress τ_o is less than the octahedral shear strength K_o. No viscoplastic creep takes place in this state. The VE strain can be directly identified using the results from creep testing (Serata et al., 1991). The time-dependent strain resulting from viscoelastic creep can best be described by a set of three or more Kelvin components as:

$$\dot{\gamma}^{VE}_{total} = \dot{\gamma}^{VE}_{23} + \dot{\gamma}^{VE}_{22} + \dot{\gamma}^{VE}_{21} \quad (3)$$

$$= (\tau_o/V_{21}) \exp(-G_{21}t/V_{21}) + (\tau_o/V_{22}) \exp(-G_{22}t/V_{22})$$

$$+ (\tau_o/V_{23}) \exp(-G_{23}t/V_{23})$$

where: $\dot{\gamma}^{VE}_{21}$, $\dot{\gamma}^{VE}_{22}$, $\dot{\gamma}^{VE}_{23}$ = short-, medium-, and long-term viscoelastic strain rates; G_{21}, G_{22}, G_{23} = retarded shear moduli for short-, medium- and long-term VE strains; V_{21}, V_{22}, V_{23} = elastoviscosity coefficients for short-, medium- and long-term VE strains.

In a similar manner, the volumetric viscoelastic strain ε^{VE}_m is given by a single Kelvin component as:

$$\dot{\varepsilon}^{VE}_m = (\sigma_m/D_2)\ [\exp(-K_2t/D_2)] \quad (4)$$

where: D_2 = hydrostatic elastoviscosity, and K_2 = retarded bulk modulus.

Viscoplastic analysis

The viscoplastic state is defined as the state at which the τ_o value is equal to or greater than K_o. In this state, the failure strength increases in proportion to the plastic strain rate. An infinite number of failure strengths can therefore exist in this state depending on the current strain rate. The viscoplastic strain rate $\dot{\gamma}^P_o$ is defined by the relation:

$$\dot{\gamma}^P_o = (K_o/V_4)\ [(\tau_o - K_o)/K_o]^n\ [(P - \sigma_m)/\sigma_m]^b\ [(T - T_o)/T_o]^L \quad (5)$$

where: V_4 = viscoplastic coefficient; P = plastic point; T, T_o = testing and absolute temperature; L = thermal coefficient of viscoplasticity; n = non-linear coefficient; b = brittle effect coefficient.

The viscoplastic creep is partly dictated by n and the brittle fracture by b. The combination of these two coefficient values determines the manner in which a given material will behave, depending on σ_m, ranging from ideal plastic flow to instantaneous explosion.

Residual strength K^R_o

During strain-softening, the strength of rock deteriorates after it has been deformed beyond the elastic limit. The ultimate destruction of the material is the state at which the intercrystalline cohesive bond is completely lost, as in a mass of loose sand. The strength K_o in this state then becomes the residual strength K^R_o, which is only the internal friction stress in the pulverized mass, given by the following function of confinement σ_m (see Fig. 3):

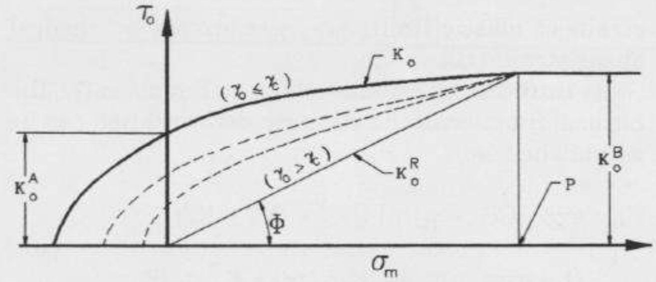

Fig. 3. Three-dimensional representation of strength of salt with regard to field surface, deterioration, and residual strength.

$$K^R_o = K^B_o\ \sigma_m/P \quad (6)$$

where: $K^B_o/P = \tan\theta$ = friction tangent; K^B_o = ultimate strength; P = plastic point; θ = angle of internal friction.

Deterioration process

Rock deterioration progresses from the intact to the pulverized strength (K_o to K^R_o) with an increase of the excess octahedral shear strain $\Delta\gamma_o$. The K_o of deteriorated rock can be found by adding the residual strength K^R_o to the variable portion ΔK_o, which varies from 0 to 100%, depending on the amount of destructive deformation. Thus the strength can be defined as:

$$K_o = f_D\ \Delta K_o + K^R_o \quad (7)$$

where: f_D = deteriorating function

ΔK_o = variable portion of the strength

$= [K^A_o + (K^B_o - K^A_o)(1 - \exp(-\alpha\sigma_m)] - K^R_o$

$K^R_o = K^B_o\ \sigma_m/P$

It is postulated that the deteriorating function changes from 0 to 1 according to the following law of natural decay:

$$f_D = e^{-x} \quad (8)$$

By relating x to $\Delta\gamma_o$, the f_D function is defined as follows:

$$f_D = \exp[-C(\gamma_o - \gamma_c)/\gamma_c] \quad (9)$$

where: C = deterioration coefficient; γ_c = critical strain of elastic limit; $\gamma_o - \gamma_c$ = excess octahedral shear strain (>0).

By introducing Equation (9) into Equation (7), the natural function of the strength deterioration can be established as:

$$K_o = \exp[-C(\gamma_o - \gamma_c)/\gamma_c]\ \{[K_o^A + (K_o^B - K_o^A)\ (1 - \exp(-\alpha\sigma_m)] - K_o\sigma_m/P\} + K_o^B\ \sigma_m/P \quad (10)$$

Figure 3 comprehensively presents the deterioration function, disclosing the brittle–ductile characteristics of the rocks sensitively manifested in the three-dimensional failure strength. It is important to note that the deterioration is characterized by one coefficient C, which can be determined in the laboratory as well as directly from field test results.

Excess (inelastic) volume expansion

The laboratory observations made by various investigators show that the dilation or non-recoverable volume expansion ε_m^N starts to increase after initiation of granular failure. The intensity of dilation, however, increases with increase of excess shear strain (γ_o–γ_c) toward a certain ultimate value. This may be expressed in the form of the natural decay function:

$$d\varepsilon_m^N = A \cdot \exp[(-\gamma_o - \gamma_c)/\gamma_c] \quad (11)$$

where: J = shear expansion coefficient; A = volume expansion constant.

Integration of Equation (11) leads to the following relation:

$$\varepsilon_m^N = F\{1 - \exp\,[-J(\gamma_o - \gamma_c)/\gamma_c]\} \quad (12)$$

where: F = maximum mean strain before total degradation at zero confinement (σ_m = 0).

The ε_m^N value decreases with an increase of plasticity or of mean stress σ_m because this non-recoverable volume expansion is caused by the brittle fracture failure processes. In the plastic state, with the mean stress larger than the plastic point P, there will be no excess volume expansion. The nonplastic effect E due to deficient lateral mean stress P – σ_m can be defined by the natural law:

$$E = \exp\,[-H\ \sigma_m/(P - \sigma_m)];\ \ \sigma_m < P \quad (13)$$

where: P = minimum σ_m value required for the strongest crystals of the grain to yield plastically; σ_m < P; H = confinement coefficient.

In Equation (13), E varies from 0 to 1 for σ_m ranging from 0 to P. The volume expansion function

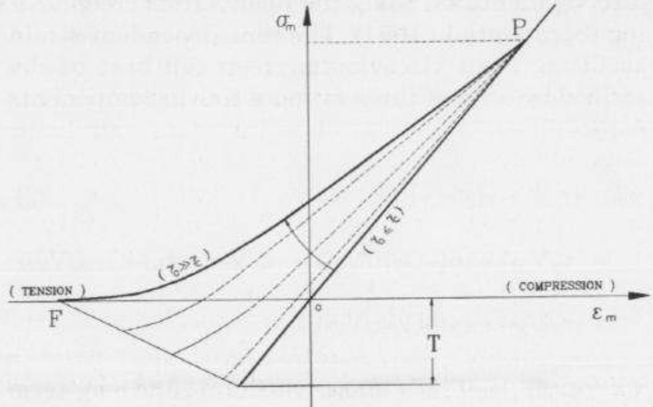

Fig. 4. Inelastic volume expansion increases as a function of excess shear strain $\Delta\gamma_o$ and mean stress σ_m.

can be formulated by multiplying Equation (12) by (13):

$$\varepsilon_m^N = F\{1 - \exp\,[-J(\gamma_o - \gamma_c)/\gamma_c]\}\ \exp[-H\sigma_m/(P - \sigma_m)] \quad (14)$$

This relation is illustrated in the mean stress–strain diagram of Fig. 4. The curve F–P indicates the ultimate volume expansion. The area between the FP and OP curves represents the conditions under which the excess volume expansion ε_m^N varies as a function of stress state and time.

Permeability function

It has been found that the increase in porosity of a deformed salt is equal to the dilation or inelastic volume expansion (Stormont and Daemen, 1991). This has led to the development of flow models in an attempt to determine the permeability of creeping salt. These transport properties of salt are of importance in evaluating the hydrological containment of storage caverns, in particular for their long-term performance. Using rock salt as a testing medium, Sandia National Laboratories has found that its permeability coefficient K is a function of excess volume expansion, minimum principal stress σ_3, and the pore structure of the medium (Stormont, 1990) as:

$$K = \beta(\sigma_3)^\lambda\ (\varepsilon_m^N)^s \quad (15)$$

where: σ_3 = minor principal stress; β,λ = empirical constants; s = constant related to pore structure.

Therefore, it is apparent that the permeability changes at each location in the ground formation according to the creep strain and stress states. The empirical constants are determined from results of laboratory flow testing (e.g., Stormont and Daemen, 1991).

FINITE ELEMENT CODE GEO

The constitutive equation derived here has been incorporated into the finite element code GEO (Geological Element Method). The GEO model can closely simulate the geomechanical and hydrological behavior of *in situ* structures under complex geometries and stress states. Preliminary comparisons between simulated results and *in situ* observations or measurements allow a rigorous assessment of the adequacy of the model's property coefficient values. Any discrepancy thus uncovered is analyzed to improve the model by adjusting the coefficient values so that the model is site-specific. *In situ* creep deformation and stress state data are particularly important for precise prediction of long-term effects. Such field calibration of the property coefficient values cannot be accomplished from results of relatively short-term laboratory testing.

The GEO computer code employs four-noded isoparametric quadrilateral elements to compute displacements, stresses, strains, and permeabilities. The program allows for axisymmetric and generalized plane–strain assumptions. The program is modular in structure so that individual subroutines can be modified or replaced without affecting the core of the program. It also provides a user-friendly interface, nodal data generation, element connectivity capability, and algorithm for bandwidth optimization. Both body forces and surface loads can be assigned to any combinations of fixed or sloping boundaries. Initial and time-dependent boundary conditions of stresses and displacements can be implemented.

DISCUSSION

Difficulties in FEM modeling of salt openings

The finite element method is a virtually perfect means of simulating behaviors of structures comprised of materials of known properties under known boundary loads, as shown in its application to spacecraft, skyscrapers, and bridges. Its application to salt structures is an entirely different matter, as we do not sufficiently know the actual *in situ* properties, stress states, and their time-dependent behavior. We have only recently begun to face this fact, which is reflected in the difficulties experienced by Sandia National Laboratories in their extensive efforts to predict the long-term behavior of the WIPP salt opening being prepared for military nuclear waste storage in the Carlsbad basin, New Mexico. The scheduled placement of nuclear waste after nearly 10 years of development and study was halted by an injunction in October 1991 until the safety of the opening can be restored. Close scrutiny of Sandia's outstanding rock mechanics studies suggests that the mathematical representation derived from laboratory test data may not result in an FEM model capable of simulating long-term behavior of salt openings. What is missing is probably the constitutive equation of the *in situ* condition, such as the one presented here. However, Sandia's laboratory test results are useful in evaluation of the constitutive equation with respect to the probable range of certain material property coefficient values.

Field calibration

A difficulty of laboratory testing for constructing the constitutive equation involves determining the effect of time on material behaviors. The time effect on long-term deterioration of salt may not be scaled down in the laboratory as can geometry effects. To assess the 10-year deterioration effect, we would have to conduct the test for ten years; such testing is not feasible. To overcome this limitation, active salt mines have been found to be an ideal test ground. In any mine, openings of various ages are readily available for immediate testing of the time effect by directly measuring the stress state (S), material properties (P), and deformation (D). Such mine measurements are essential in calibrating the constitutive equation of salt for realistic prediction of long-term behavior. The field instruments required to measure S, P, and D were successfully developed and extensively used in various salt and potash mines, enabling us to collect the data to construct the GEO model for site-specific applications. This field-based development of the constitutive equation has made the GEO model reliable. Examples of large-scale field application are given in two papers presented at this symposium, one for dry mining (Dickie et al., 1993) and one for solution mining (Mehta and Serata, 1993).

CONCLUSIONS

The constitutive equation is formulated to describe the brittle–ductile duality and long-term behavior of rock salt and other related geological materials by incorporating the field conditions, which consist of seven major behavioral components: elasticity, viscoelasticity, viscoplasticity, strength deterioration, volumetric expansion, thermal expansion, and brittle–ductile failure.

The mechanically-defined ground behavior simultaneously provides porosity increase and permeability, enabling simulation of long-term hydrological behavior. The GEO constitutive equation enables realistic modeling of long-term behavior of complex earth structures such as salt mines and solution caverns.

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