Creep Constitutive Modeling of Rock Salt and Evaluation of Model Parameters using Optimization Technique

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Introduction

ock salt exhibits creep deformation when subjected to mechanical or thermomechanical loading. Creep deformations are generally the result of various stress assisted-thermally activated micromechanisms such as generation and immobilization of dislocations, escape of dislocations from their glide planes, grain boundary sliding and diffusion of atoms and point defects (Faruque and Zaman, 1988). The primary and the secondary phases of creep are gradually dominated by the dislocation-related micro-mechanisms while the tertiary creep phase is dominated by the evolution of micro-cracks and micro-voids. The formation of micro-cracks and micro-voids results in a strong creep dilatancy observed in the tertiary phase of creep (Chen et al., 1994; Chen and Wang, 1995; Chen and Schreyer, 1994). At a given stress and temperature range, some of these micromechanisms govern the creep deformation process. In the past, various constitutive models have been developed to describe creep response of rock salt. These models can be broadly categorized as phenomenological, viscoelastic, viscoplastic, and micromechanical (Faruque and Zaman, 1990). Most of the above-mentioned creep models assume the existence of a creep potential applicable to a stress and temperature range. Consequently, model-predicted creep strain rates do not agree with experimental observations at all levels of stress and

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temperature. The constitutive model presented in this paper assumes dislocation-related micromechanisms as the primary sources of creep and thereby characterizes primary and secondary phases of creep deformation only. The proposed model does not account for damage evolution generally observed during the transition from the secondary to the tertiary creep phase. The constitutive model is formulated using the concept of piecewise linearity in the effective stress-creep strain rate relationship. Effective stress at a point is simply the difference between the applied stress and the back stress. Since the piecewise linearity is assumed, an explicit functional form is not needed to predict the creep strain rate. Therefore, creep strain rate can be accurately predicted by this model for a wide range of stress and temperature.

Objective

The main objective of this paper is to present a rate-dependent constitutive model to describe the creep behavior of rock salt. The model developed in this study is based on the dislocation-related micromechanisms. The associated five model parameters are evaluated using an optimization technique. It is also intended to demonstrate how an optimization technique can help significantly in improving the creep response prediction of rock salt. The developed model is used for the prediction of creep response of rock salt under thermomechanical loadings and the results are compared with the experimental data.

Need for Modeling the Creep Deformation of Rock Salt

Creep or time-dependent deformation of rock salt is a very important property from a waste repository consideration. Since rock salt is considered as a prime candidate for nuclear waste repository, it is important to study the creep behavior of rock salt under different thermomechanical conditions. Temperatures, even near to a canister of high level waste, needs to be kept well below those sufficient to produce any radical changes in the structural properties of rock salt (the melting temperature is about 800°C). Heating enhances the ability of salt to undergo viscoplastic deformation without failure, both under tensile and compressive stresses. For the probable repository conditions of relatively low to medium temperatures (25°C to 100°C in the near field, and perhaps 300°C adjacent to a waste package) and low to moderate stresses (0 to 20 MPa), salts have demonstrated high potential for significant creep deformation (Senseny, 1983; Zaman, 1986). Evaluation of such creep deformation and recrystallization behavior is important in overall performance assessment (PA) of a repository in salt.

The development of creep constitutive models are, therefore, important to characterize the creep response of rock salt under mechanical and thermal loadings for a safe and economical design of structures and facilities in rock salt. It is essential that the constitutive laws which are based on a phenomenological approach account for the important mechanisms which govern the creep response of a material in formulating such constitutive equations.

Brief Review of Literature

Creep Modeling

Many researchers in the past have presented and reviewed (Cristescu. 1992; Cristescu, 1993; Senseny, 1983; Zaman et al., 1992; Zaman, 1986) various creep laws used to describe creep response in rock salt in mining operation and in nuclear waste repository. The constitutive models, based on phenomenological or micromechanical framework (Garafalo, 1965; Robotnov, 1969; Odqvist, 1974; Krieg et al., 1978; Robinson, 1978; Henderson, 1979; Kraus, 1980) generally assume the creep strain rate to be a specified function of the applied stress, the elapsed time after the application of the stress and sometimes, the current temperature. However, experimental facts (Blass, 1971) indicate that creep is an intrinsically anisotropic phenomenon governed by the past history of deformation. A change in the direction of the stress vector causes a transient softening of the material for a certain range of the succeeding strain. It is always possible to represent the deformation history by the strain trajectory in the creep strain space. The above phenomena, in turn, specifies the range of temporary softening of the material by certain closed surface in the creep strain space. Furthermore, the experimental results show a transient non-coaxiality between the stress tensor and the creep rate tensor due to an abrupt change in the direction of the stress tensor (Mroz, 1969; Murakami and Ohno, 1982). As a result, these types of models encounter difficulties in accurately predicting the instantaneous increase in the creep strain rate for reversal of stresses (Faruque and Zaman, 1988; Mahmood et al., 1989). Some internal variables related to physical mechanisms are, therefore, needed in the constitutive model to accurately describe creep responses under such situations. A widely used internal variable called the back stress, associated with the dislocation pileups, is used in the proposed model. Incorporation of back stress enables the model to predict both transient and steady state creep response of polycrystalline solids under complex stress and temperature histories.

Optimization Techniques

A model contains several material constants which can broadly be classified as 'fixed' and 'free' parameters. The parameters which can be determined from simple laboratory tests are defined as 'fixed parameters'; the remaining parameters are the 'free parameters'. The 'free' parameters are established by curve fitting (Senseny, 1993) or by trial-and-error with the objective being to obtain the best overall fit to a given experimental data or set of observed responses. There are many optimization techniques available in the literature to evaluate an optimal set of values for the 'free' parameters of a model (Box, 1955; Box, 1965; Pierre, 1969; Murray, 1972; Fletcher, 1987). Various classes of minimization procedures are available to direct the search for minimization. Among others, direct search method which applies both the 'simplex approach' and 'complex approach' are widely used in the optimization of material constants. Because of the simplicity and great generality of the simplex approach, it has proven to be quite reliable in practice (Swann, 1972) and is chosen for this study. As a result, this approach is implemented into a workable computer code.

Micromechanical Processes Involved in the Proposed Model

The creep characteristics of rock salts are the result of a number of micromechanical processes such as vacancies and diffusion; dislocations and slip; and grain boundaries defects and recrystalization (Evans, 1985; Hossain, 1992). The governing mechanisms for polycrystalline materials, such as rock salts, include:

- stress assisted and thermally activated migration of defects past obstacles;
- 2. generation and immobilization of dislocations leading to an increase in the dislocation density and dislocation pileups; and,
- stress assisted and thermally activated rearrangements of dislocations (Faruque, 1988).

Since micromechanical processes primarily control the creep mechanism, it is necessary to incorporate some internal variables, in addition to the external stress and temperature histories, to the creep constitutive models. One of such internal variable is the back stress tensor (interdislocation internal stress) that is associated with the dislocation pileups due to applied stress tensor (σ_{ij}) and temperature (T). The difference between the applied deviatoric stress tensor (S_{ij}) and the deviatoric back stress tensor (α_{ij}) is often termed as the 'effective stress' tensor (τ_{ij}), i.e.

$$\tau_{ij} = S_{ij} - \alpha_{ij} \tag{1}$$

It may be noted that the deviatoric back stress (α_{ij}) is controlled by the dislocation related time-dependent internal processes and, therefore, is a function of time. There will be no back stress initially when a stress (σ_{ij}) is

applied to a virgin material. The back stress builds up gradually with time as the creep deformation continues. Consequently, the effective stress (τ_{ij}) decreases continuously with time (if the applied stress is held constant) due to the gradual increase of the back stress.

Proposed Creep Model for Rock Salt

It is postulated by Faruque and Zaman (1988) that the creep strain rate tensor, $\dot{\varepsilon}_{ij}^{c}$, is a unique function of the effective stress tensor, τ_{ij} , and therefore, can be expressed as

$$\dot{\varepsilon}_{ij}^{c} = f_{ij}(\tau_{ij}) \tag{2}$$

where the response function f_{ij} is a tensor valued function of the single tensor argument τ_{ij} . As experimental evidence suggests, it is reasonable to assume that the principal directions of $\dot{\varepsilon}_{ij}^{c}$ are coincident with the principal directions of τ_{ij} (Zaman et al., 1992). Using this condition and the representation theorem of Rivlin and Ericksen (1955), the following expression can be written:

$$\dot{\varepsilon}_{ij}^{c} = f_{1} \tau_{ij} \tag{3}$$

The scaler response function f_1 depends upon the invariants of τ_{ij} . Since τ_{ij} is assumed to be deviatoric, it has only two independent invariants, I_2 and I_3 , as follows

$$I_2 = 1/2 \left(\tau_{ij} \cdot_{ji} \right) \tag{4}$$

$$I_3 = \frac{1}{3} \left(\tau_{ij} \tau_{jk} \tau_{ki} \right) \tag{5}$$

In the inviscid theory of plasticity for polycrystalline materials, the yield function is defined in terms of the second invariant of the deviatoric stress tensor only (Faruque and Zaman, 1990). Assuming similar representation for creep, the function f_1 can be expressed in the form

$$f_1 = 3/2 \left\{ a \left(3 \cdot I_2 \right)^{n/2} \right\}$$
(6)

where a and n = material constants.

Factors 3/2 and 3 are used in Eqn. (6) to maintain consistency between 3-D

and uniaxial cases, of the function f_i . The expression for ε_{ij}^c , in view of Eqn.s (3) and (6) can be written in an explicit form as

$$\dot{\varepsilon}_{ij}^{c} = (3/2) \left\{ a (3I_2)^{n/2} \tau_{ij} \right\}$$
 (7)

In general, the deviatoric back stress at saturation, α_{ij}^{s} , is a function of the applied deviatoric stress (S_{ij}) and the temperature (T) and can be expressed as

$$\alpha_{ij}^{s} = h_{ij}(S_{ij}, T)$$
(8)

The function $h_{ij}(S_{ij}, T)$ has a second order tensor argument. Assuming α_{ii}^{s} to be linear in S_{ij} , it can be expressed in the following form

$$\alpha_{ij}^{s} = h_1 S_{ij} \tag{9}$$

According to the representation theorem (Rivlin and Ericksen, 1955), h_1 is a function of the invariants J_2 and J_3 of the deviatoric stress tensor S_{ij} and temperature (T). As described before, the yield function is defined in terms of the second invariant (J_2), where

$$J_{2} = (1/2)(S_{ij}S_{ji})$$
(10)

 h_1 and α_{ii}^s can be expressed as

$$h_{1} = g(T) (3J_{2})^{m/2}$$
(11)

$$\alpha_{ij}^{s} = g(T) (3J_{2})^{m/2} S_{ij}$$
(12)

In Eqn.s (11) and (12) 'm' is a material constant and g(T) is a function that accounts for the effect of temperature on the value of α_{ij}^{s} . The function g(T) is capable of describing the isothermal creep at different temperatures and assumes the form

$$g(T) = 1 - \overline{b} * \exp(-Q/RT)$$
(13)

where,

 \overline{b} = modified material constant of 'b'; Q = activation energy; R = universal gas constant; and

T = temperature in °K.

For given temperature, g(T) can be replaced by a constant 'b' and Eqn. (13) can be written as,

$$b = 1 - \overline{b} * \exp(-Q/RT)$$
(14)

The evolution of α_{ij} is controlled by strain hardening due to immobilization and pilingup of dislocations at a barrier and by viscous recovery due to the escape of dislocations from their glide planes. Assuming (Faruque and Zaman, 1990) that the evolution of α_{ij} is governed by the law of kinetics, $\dot{\alpha}_{ij}$ can be written as,

$$\dot{\alpha}_{ij} = y_{ij} \left(v_{ij} \right) \tag{15}$$

where the response function y_{ij} is a tensor function of the unit tensor argument (v_{ij}) , in which v_{ij} can be written as

$$\nu_{ij} = \frac{\left(\alpha_{ij}^{s} - \alpha_{ij}\right)}{\left\|\left(\alpha_{ij}^{s} - \alpha_{ij}\right)\right\|}$$
(16)

The symbol $\|\cdot\|$ in Eqn. (16) denotes quadratic norm of the argument tensor. It may be noted that the second order tensors α_{ij} , α_{ij}^{s} and $\dot{\alpha}_{ij}$ are all deviatoric.

Assuming that $\dot{\alpha}_{ij}$ and ν_{ij} are colinear, one can write

$$\dot{\alpha}_{ij} = \frac{d \alpha_{ij}}{d t} = \sqrt{\frac{2}{3}} \left\{ c (3k_2)^{u/2} v_{ij} \right\}$$
(17)

$$y_{1} = \sqrt{\frac{2}{3}} \left\{ c \left(3 k_{2} \right)^{u/2} \right\}$$
(18)

where

$$\mathbf{k}_{2} = \left(\alpha_{ij}^{s} - \alpha_{ij}\right) \left(\alpha_{ji}^{s} - \alpha_{ji}\right)$$
(19)

.

and

where c and u = material constants.

Specialized Form of the Proposed Creep Model for Triaxial Loading

In order to verify the capability of the model and simplify the working equations, the model is specialized for triaxial loading path to predict the creep behavior of rock salt. A material under triaxial loading condition will have an axial stress of σ_{11} and a confining stress of σ_{22} (= σ_{33}).

For this specialized multiaxial loading, Eqs. (12), (17) and (7) can be written, respectively, as

$$\alpha_{11}^{s} = b(\sigma_{11} - \sigma_{22})^{m+1}$$
(20)

$$\dot{\alpha}_{11} = c \left[\left(\alpha_{11}^{s} - \alpha_{11} \right) - \left(\alpha_{22}^{s} - \alpha_{22} \right) \right]^{u}$$
 (21)

$$\dot{\varepsilon}_{11}^{c} = \mathbf{a} \left[\left(\sigma_{11} - \sigma_{22} \right) - \left(\alpha_{11} - \alpha_{22} \right) \right]^{n+1}$$
 (22)

Evaluation of Model Parameters

The proposed model contains a total of six parameters, namely, a, b, c, m, n and u. In this study, creep test data for Avery Island Dome salt is used to evaluate the model parameters and to validate the model through back prediction of test data. From exploratory analyses of data, 'm' was found to be negligible and is therefore assumed as zero (Hossain, 1992). As such, there are only five independent parameters to be evaluated for the dome salt.

Steps Involved in Evaluation of Creep Strain Using the Proposed Model

The simplified form of the model for triaxial loading can be used to calculate the creep strain of polycrystalline materials, such as rock salt. The following steps are followed to achieve this objective.

- (1) At the beginning, initialize the model by setting the starting values of α_{ij}^{s} , $\dot{\alpha}_{ij}$, $\dot{\varepsilon}_{ij}^{c}$ and ε_{ij}^{c} to zero. The values at the end of a given cycle become the starting values for the beginning of the next cycle.
- (2) Calculate the saturated internal back stress (α_{ii}^{s}) from Eqn. (20).
- (3) Calculate the internal back stress rate $(\dot{\alpha}_{ij})$ from Eqn. (21). The other components of the Eqs. are already known. The increment in the internal back stress $(\Delta \alpha_{ij})$ at a particular time is calculated using the Runga-

Kutta Method. The current internal back stress is determined by adding the previous internal back stress and the incremental internal back stress pertaining to the incremental time.

(4) Calculate the creep strain rate $(\dot{\varepsilon}_{ij}^{c})$ from Eq. (22). The incremental creep strain $(\Delta \varepsilon_{ij}^{c})$ at a particular time can be calculated by using three point numerical derivative formula. The current creep strain is the addition of previous creep strain and the incremental creep strain.

A computer program is developed to calculate the creep strain using the steps outlined above. The creep strain at very small time intervals and for any number of loading steps can be predicted by using this computer code (Hossain, 1992).

The Optimization Process

An optimization process is a technique to identify a set of values of the associated parameters which would enable the constitutive model to most closely simulate the observed material response. This goal is usually achieved when the 'error function' assumes an optimal (i.e. a maximum or a minimum) value. The task of model calibration is readily cast in the form of a minimization problem.

The 'error function' is the summation of residuals of all experimental data and the corresponding model predictions (Fig. 1). The residual at a point



FIGURE 1 : Definition of an 'Error Function'

is considered as the scalar discrepancy between the model prediction and the experimental observation at that point. The total residual for a calibration dataset can be obtained by summing up all the residuals corresponding to all the experimental data points. Mathematically

ERR =
$$\frac{\sum_{i=1}^{k} (Y_{ie} - Y_{ip})^{2}}{\sum_{i=1}^{k} Y_{ie}^{2}}$$

(23)

where

k = number of points on the time axis at which the vertical error is calculated;

 Y_{ip} = creep strain values predicted by the model; and Y_{ie} = creep strain values as obtained experimentally.

In order to completely generalize the error function formation process, it is possible to apply different weights to specific components (e.g., loading/ unloading or primary/steady-state part of the experimental data) of a dataset. For example, by assigning a given observation a weight of zero, it is possible to exclude that part in the dataset, without influencing the computed value of the error function and, therefore, the final form of the calibrated model. Thus, the differential weighing option makes it easy to investigate the effect of various components of an experimental dataset on the final computed 'optimal' solution.

Optimization Process using 'Box Algorithm'

An optimization algorithm ideally seeks to locate the error function's 'global minimum' – namely that set of parameter values for which the function assumes its minimum value. A set of parameter values is said to achieve global minimum only when it gives the same set of parameter values irrespective of the initial points from where the search for minimum point is initiated. Only for certain special cases of functions, this goal of global minimization can normally be achieved. Extreme difficulties are encountered in developing algorithms that can locate the global minima of error functions encountered in many practical optimization algorithms can only locate a 'local minimum' in the vicinity of the initial search region. In most practical problems, the degree of global uniqueness and global unimodality can only be indirectly estimated (DaNatale, 1983). Normally, this is accomplished by initiating the search from several different starting points in the n-dimensional parameter space and then comparing the various solutions. If the searches all

converge to the same point, the error function is probably unimodal in the domain of interest, with the point of convergence thus representing the global minimum. If the searches fail to converge to the same point, the error function is clearly non-unimodal in the space of concern. Provided that a sufficient number of trials have been performed, the point in space associated with the absolute lowest function value may thus be presumed to be the global minimum.

Nearly all methods developed to locate the minimum of a general nonlinear function are iterative in nature. If the initial estimate of the solution is given, they proceed by generating a sequence of new estimates, each of which represents an improvement over the previous ones. The various optimization procedures are thus distinguished by the particular strategies employed to produce this series of improving approximations that finally lead to the identification of an acceptable minimum. During the iterative search, the domain of acceptable solutions is continuously reduced. In the most efficient algorithms, this reduction is accomplished through a combination of sectioning (such as simple bisection) and interpolation (in which a polynomial of some particular order is first fitted to known data and then analytically minimized to yield the subsequent trial point). The search may be guided by varying degrees of data, including function values as well as perhaps gradient and curvature information.

The number of evaluations needed to locate a function's minimum is, in general, strongly dependent on the distance from that point at which the search is started. Hence, in establishing the merits of a given problem characterization, it is also necessary to consider the relationship between the error in the starting estimate and the number of function evaluations required.

Direct Search Method

Several methods are currently available for function minimization among which the direct search methods have been found to be very effective for evaluation of material constants for a given constitutive model (Box, 1965; Swann, 1972). In the direct search approach, the n-dimensional solution space is generally explored by defining a set of directions and then searching along each direction in a cyclical manner. The 'Simplex Approach' introduced by Spendley et al. (1962) is one of the most successful direct search algorithm. The procedure is based on the evolutionary operation (EVOP) technique originally introduced by Box in 1955. In this approach the solution space is explored by means of a geometrical configuration of points rather than a set of directions. A number of modifications to this basic approach have since been suggested, but the version by Nelder and Mead (1965) is commonly regarded as the most effective. In this version, the simplex automatically rescales itself according to the local geometry of the error function. The direct search method using 'Box Algorithm' is able to operate problems with many constraints. It also does not require any derivative form of the error function and constraints. The operating principle of 'Box Algorithm' consists of initialization of parameter values, reflection, feasibility of reflection point, and check for termination of the optimization (Hossain, 1992).

In view of the difficulties and complexities associated with establishing global minimum of the error function, a large number of trials may be required for different starting search regions to get a global minimum or at least 'strong' local minimum points. In the present work, several trials were given for each data set and the code was run on double precision to control the possible numerical problems.

Results and Discussions

General

The model presented in the preceding section is used to predict the creep behavior and the results are compared with the laboratory tests on Avery Island Dome salt (Mellegard, 1983). The model parameters are selected by using an optimization technique. Table 1 shows the experimental data set identification number along with the temperature, confining pressure and deviatoric stress used in the creep tests.

Optimization of Model Parameters and Back Prediction

The model parameters are optimized in a stepwise manner so as to observe the predictive capabilities of the model and the optimization process. The quality of prediction is assessed using a numerical scheme, as presented in Table 2.

In the first step, one single data set is optimized using the optimization technique discussed previously. The model parameters thus obtained are used to predict the same data set that is used for optimization as well as additional data sets that are not used for parameter optimization. Figures 2 and 3 show the comparison of creep strain vs. time for experimental and predicted values. The model parameters obtained from the optimization of a single data set is able to predict the same data set extremely well (Fig. 2). The prediction can be relatively poor with the same parameter set when used to predict an 'unoptimized data' set as can be seen in Fig. 3. The prediction can become even worse as is seen in Fig. 4.

Therefore, an attempt is made to improve the overall predictive capabilities of the model by using multiple data set for evaluation of the model parameters in an optimum manner. Three sets of laboratory test data

Identification	Temperature	Confining	Deviatoric Stress (MPa)	
Number	(°C)	Pressure (MPa)		
C247	C247		10.3	
D249		3.4	6.9	
T242	24	3.4	10.3	
D244		3.4	20.7	
T245		20.7	10.3	
T702	70	3.4	10.3	
T705		20.7	10.3	
T1003		3.4	10.3	
D10012		13.8	5.0	
D1008		13.8	12.1	
D1007		13.8	13.8	
D10011	100	13.8	17.2	
D1005	100	13.8	20.7	
D10022		15.0	9.0	
D10020		15.0	12.5	
D10014		15.0	15.0	
T1001		20.7	10.3	

Table 1 : Identification Number of Rock Salt Data Sets used in This Study

 Table 2

 Range of Error Levels to Define the Prediction

 Quality of Rock Salt Data

Prediction Quality	Error Level		
Excellent	< 1.0E-3		
Very Good	1.0E-3 to 5.0E-3		
Good	5.0E-3 to 5.0E-2		
Poor	> 5.0E-2		



FIGURE 2 : Good Back Prediction of Experimental Creep Strain of a Data Set (# D1008) used in Parameter Optimization



FIGURE 3 : Good Prediction of a Data Set (# D1007) not used for Single Data Set Optimization



FIGURE 4 : Poor Prediction of a Data Set (# D10011) not used for Single Data Set Optimization



FIGURE 5 : Comparison of Experimental and Predicted Creep Strain for a Data Set (# D10011 – used fer Multiple Data Set Optimization) using the Final Parameter Set.



FIGURE 6 : Comparison of Experimental and Predicted Creep Strain for a Data Set (# D1702 – not used for Multiple Data Set Optimization) using the Final Parameter Set.

are used for parameter optimization. The final set of parameter values thus obtained for Avery Island dome salt are as follows:

c = 0.60E-1;
a = 0.40E-6;
n = 2.00;
b = 0.981 (for temp. =
$$24^{\circ}$$
C);
= 0.893 (for temp. = 70° C);
= 0.728 (for temp. = 100° C); and
u = 3.06.

Using these parameter values a number of experimental data sets, that are either used or not used for parameter optimization, are predicted using this model. Fig. 5 represents the back prediction of data set D1008 which was used for parameter optimization using multiple data sets. On the other hand, Fig. 6 shows the prediction of data set D1007 which was not used for parameter optimization. The predictions are very good and encouraging in both cases. Therefore, it is quite clear that the parameters obtained from the optimization with multiple data set are more representative and can improve the predictive capability of the model significantly. Table 3 gives the summary of test number, optimization combination of data set and prediction quality.

Data Set	Type of Optimization	Parameter Values	Data Set Used for Prediction	Error	Prediction Quality
D1008	Single Data Set	c = 0.58E-1 a = 0.86E-6 n = 1.60 b = 0.74 u = 2.75	Optimized	1.94E-4	Excellent
D1007			Unoptimized	1.36E-2	Good
D10011			Unoptimized	1.09E-1	Poor
D1005			Unoptimized	2.05E-1	Poor
D10012	Multiple Data Set	c = 0.10 a = 0.36E-6 n = 1.77 b = 0.74 u = 1.70	Optimized	1.06E-2	Good
D10011			Optimized	5.07E-3	Very Good
D1008			Optimized	1.62E-2	Good
D1007			Unoptimized	9.15E-3	Good
D1005			Unoptimized	1.48E-2	Good

Table 3 : Prediction Quality of Rock Salt Data with Final Parameter Set

Concluding Remarks

Creep deformations in rock salt are generally the result of various stress assisted-thermally activated micromechanisms such as generation and immobilization of dislocations, escape of dislocations from their glide planes, grain boundary sliding and diffusion of atoms and point defects. At a given stress and temperature range, some of these micromechanisms govern the creep deformation process.

A rate dependent constitutive model based on 'effective stress' approach is presented here to describe the creep deformation of polycrystalline material, namely, rock salt. The model is used to predict and compare the creep strain of Avery Island Dome salt. The direct search methods, of which the simplex approach of function minimization is the most successful, is used here for the evaluation of 'free parameters' of the model in an optimal manner. The number of evaluations needed to locate a function's global minimum is, in general, strongly dependent on the initial search point. In view of the difficulties and complexities associated with establishing global minimum of the error function, a large number of trials are required from different starting points to get a global minimum or at least a 'strong' local minimum point. In this study, the associated five parameters of the model are evaluated with sufficient number of trials to get at least a strong local minimum point. In the process of optimization, experimental data for rock salt is first employed for optimization of model parameters. The model parameters optimization is carried out in two ways: single data set optimization and multiple data set optimization. The optimized parameters are then utilized to predict the creep of data sets not used for optimization. It is found that for the parameters obtained from single data set, optimization can back predict the same data set in an excellent manner. But the predicted response can exhibit a difference compared with the experimental data when using an 'unoptimized data' set. On the other hand, the parameters obtained from multiple data set optimization can predict the creep response quite well for both optimized as well as unoptimized data sets. It is, thus, found that use of optimization technique can improve the prediction quality of creep response obtained from the use of the constitutive model.

Bibliography

BLASS, J.J. and FINDLEY, W.N. (1971) : "Short-Time Biaxial Creep of an Aluminum Alloy with Abrupt Change of Temperature and State of Stress", *ASME J. of Appl. Mech.*, 38, pp.489-492.

BOX, G.E.P. (1955) : "Evolutionary Operation: A Method for Increasing Industrial Productivity", Paper presented to the International Conference on Statistical Quality Control, Paris, July 1955. Reproduced in *Applied Statistics*, Vol.VI, pp.3-22, 1957.

BOX, M.J. (1965) : "A New Method of Constrained Optimization and a Comparison with Other Methods", *Comput. J.*, Vol.8, pp.42-52.

CHEN, Z., WANG, M.L., MIAO, S., and LU, T. (1994) : "Study of Rock Salt Creep via a Viewpoint of Phase-Transition", *Proc. 4th Annual WERC Technology Development Conference*, DOE/WERC, Las Crus, New Mexico, pp.181-190.

CHEN, Z. and WANG, M.L. (1995) : "Some Recent Advances in Modeling Rock Salt Creep", *Numerical Models in Geomechanics — NUMOG V*, Eds. Pande and Pietruszczak, Davos, Switzerland, Sept. 1995, pp.9-14.

CHEN, Z. and SCHREYER, H.L. (1994) : "On Nonlocal Damage Models for Interface Problems", Int. J. of Solids and Structures, Vol.31, No.9, pp.1241-1261.

CRISTESCU, N. (1992) : "Constitutive Equation for Rock Salt and Mining Applications", *Seventh Int. Symp. on Salt*, Vol.1, Elsevier Sci. Publ., Amsterdam, pp.105-115.

CRISTESCU, N. (1993) : "A General Constitutive Equation for Transient and Stationary Creep of Rock Salt", *Int. J. Rock Mech. Min. Sci.*, Vol.30, No.2, pp.125-140.

DANATALE, J.S. (1983) : "On the Calibration of Constitutive Models by Multivariate Optimization. A Case Study: The Bounding Surface Plasticity Model", *Ph. D. Thesis*, University of California, Davis.

EVANS, R.W. and WILSHIRE, B. (1985) : Creep of Metals and Alloys, The Inst. of Metals, London.

FARUQUE, M.O. and ZAMAN, M.M. (1990) : "A Thermo-mechanical Creep Constitutive Model for Metals with Application", *Proceedings of the Composite Material Technology*, The 13th Annual Energy Sources Technology Conference and Exposition, New Orleans, Louisiana, pp.173-176.

FARUQUE, M.O. and ZAMAN, M.M. (1988) : "On Modelling Steady State and Transient Creep of Polycrystalline Solids", *Acta Mechanica*, 71, pp.115-136.

FLETCHER, R. (1987) : Practical Methods of Optimization, 2nd Edition, John Wiley and Sons, Chichester, U.K.

GARAFALO, F. (1965) : Fundamentals of Creep and Creep-Rupture in Metals, Macmillan, New York.

GILL, P.E. and MURRAY, W. (1974) : Numerical Methods for Constrained Optimization, Academic Press.

HENDERSON, J. (1979): "An Investigation of Multiaxial Creep Characteristics of Metals", ASME J. of Eng. Mat. and Tech., Vol.101, pp.356-364.

HOSSAIN, M.I. (1992) : "A Preliminary Creep Model for Avery Island Dome Salt for Nuclear Waste Repository Application", *M.S. Thesis*, University of Oklahoma, Norman, Oklahoma.

KRAUS, H (1980) : Creep Analysis, John Wiley and Sons, Inc., New York.

KRIEG, R.D., SWEARENGEN, J.C. and RHODE, R.W. (1978) : "A Physically Based Internal Variable Model for Rate-Dependent Plasticity", *Inelastic Behavior* of *Pressure Vessel and Piping Components*, T.Y. Chang, and E. Krempl eds., pp.15-28.

MAHMOOD, I.U., FARUQUE, M.O. and ZAMAN, M.M. (1989) : "Application of an Internal Variable Constitutive Model to Predict Creep Response of an Aluminum Alloy Under Multiaxial Loading", *ASME J. of Appl. Mech.*, 56, pp.514-518.

MELLEGARD, K.D. and SENSENY, P.E. (1983) : "Exponential-Time Creep Law for Avery Island Salt", *ONWI-329*, Prepared by RE/SPEC Inc. for Office of Nuclear Waste Isolation, Battelle Memorial Institute, Columbus, Ohio.

MROZ, Z. (1969) : "An Attempt to Describe the behavior of Metals Under Cyclic Loads Using a More General Workhardening Model", *Acta Mechanica*, 7, pp.199-205.

MURAKAMI, S. and OHNO, N. (1982) : "A Constitutive Equation of Creep Based on the Concept of a Creep-Hardening Surface", *Int. J. of Solids and Structures*, 18, pp.597-609.

MURRAY, W. (1972a) : "Fundamentals", Numerical Methods for Unconstrained Optimization (W. Murray, ed.): Academic Press, London, U.K., pp.1-12.

NELDER, J.A. and MEAD, R. (1965) : "A Simplex Method for Function Minimization", *Computer J.*, Vol.7, pp.308-313.

ODQVIST, F.K.G. (1974) : Mathematical Theory of Creep and Creep Rupture, Oxford University Press.

PIERRE, D.A. (1969) : Optimization Theory with Applications, John Wiley and Sons, Inc.

RIVLIN, R.S. and ERICKSEN, J. (1955) : "Stress Deformation Relations for Isotropic Materials", J. of Rational Mech. Anal., Vol.4, pp.323-425.

ROBOTNOV, Y.N. (1969) : Creep Problems of Structural Members, North Holland, Amsterdam.

ROBINSON, D.N. (1978) : "A Unified Creep-Plasticity Model for Structural Metals at High Temperature", *ORNL/TM-5969*, Oak Ridge National Laboratory.

SENSENY, P.E. (1983) : "Review of Constitutive Laws Used to Describe the Creep of Salt", *RSI-0151*, Prepared by RE/SPEC Inc., Rapid City, SD for Office of Nuclear Waste Isolation, Battelle Memorial Institute, ONWI-295.

SENSENY, P.E., BRODSKY, N.S. and DEVRIES, K.L. (1993) : "Parameter Evaluation for a Unified Constitutive Model", *ASME, J. of Eng. Mat. and Tech.*, Vol.115, pp.157-162.

SPENDLEY, W., HEXT, G.R. and HIMSWORTH, F.R. (1962) : "Sequential Application of Simplex Designs in Optimization and Evolutionary Design", *Technometrics*, Vol.4, pp.441-461.

SWANN, W.H. (1972) : Direct Search Methods in Numerical Methods for Unconstrained Optimization, W. Murray Edition, Academic Press, London, U.K., pp.13-28.

ZAMAN, M. (1986) : "Assessment of Constitutive Models for Salt Creep in a Waste Repository Environment", *Draft Report*, Argonne National Laboratory Report, Argonne, Illinois.

ZAMAN, M., FARUQUE, M.O. and HOSSAIN, M.I. (1992) : "Modeling Creep Behavior of Rock Salt", *Proceedings of the Energy Technology Conference and Exposition (ETCE)* : Houston, Texas, January 1992, Published in Composite Material Technology Section, PD-Vol.45, ASME, pp.51-56.