CONSTITUTIVE BASIS OF THE MDCF MODEL FOR ROCK SALT

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ABSTRACT

All valid constitutive equations must satisfy two general invariance principles as well as several other principles. In this paper, the MDCF (Multimechanism Deformation Coupled Fracture) model for rock salt is shown to be thermodynamically consistent, coordinate invariant, frame indifferent, and physically admissible. Additionally, the stress rates used in the formulation are shown to be kinematically consistent with the Cauchy stress rates.

MDCF MODEL

In the MDCF formulation (Chan *et al.* [1992], [1994],[1996a], [1996b]), the Green-Naghdi stress rate (Johnson & Bammann [1984]) is given as a function of the difference between the rate-of-deformation tensor, D and the inelastic rate-of-deformation tensor, D^I.[2] The latter is decomposed into contributions from various deformation mechanisms and is described by the generalized kinetic equation (Chan *et al.* [1996a]),

$$D^I = \frac{\partial \sigma_{eq}^c}{\partial T} \dot{\varepsilon}_{eq}^c + \frac{\partial \sigma_{eq}^{\omega_s}}{\partial T} \dot{\varepsilon}_{eq}^{\omega_s} + \frac{\partial \sigma_{eq}^{\omega_t}}{\partial T} \dot{\varepsilon}_{eq}^{\omega_t} \tag{1}$$

where T, σ_{eq}^c, $\sigma_{eq}^{\omega_s}$, $\sigma_{eq}^{\omega_t}$, $\dot{\varepsilon}_{eq}^c$, $\dot{\varepsilon}_{eq}^{\omega_s}$, $\dot{\varepsilon}_{eq}^{\omega_t}$ are Cauchy stress, conjugate equivalent stress measures and equivalent inelastic rates of deformation for dislocation creep (c), shear damage (ω_s), and tensile damage (ω_t) mechanisms, respectively. The conjugate equivalent stress measures play the role of flow potentials for each deformation mechanism, and the derivative with Cauchy stress gives the flow direction. The equivalent inelastic rates of deformation play the roles of kinetic functions. Damage development is modeled with the use of the Kachanov

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[1] A Department of Energy Facility
[2] Throughout the text, bold-face type will be used to denote a vector or tensor.

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damage variable (Kachanov [1958]) determined from an evolution equation. The functional dependencies of the various MDCF components are as follows.

$$\sigma_{eq}^c = \Sigma^c(T_1, T_3), \quad \sigma_{eq}^{\omega_s} = \Sigma^{\omega_s}(I_1, T_1, T_3), \quad \sigma_{eq}^{\omega_t} = \Sigma^{\omega_t}(T_3)$$

$$\dot{\varepsilon}_s = E_s(\sigma_{eq}^c, \omega, \Theta), \quad \dot{\varepsilon}_{eq}^c = E^c(\sigma_{eq}^c, \zeta, \omega, \Theta), \quad \dot{\varepsilon}_{eq}^{\omega_s} = E^{\omega_s}(\sigma_{eq}^{\omega_s}, \omega, \Theta), \quad \dot{\varepsilon}_{eq}^{\omega_t} = E^{\omega_t}(\sigma_{eq}^{\omega_t}, \omega, \Theta) \quad (2)$$

$$F = F(\zeta, \sigma_{eq}^c, \omega, \Theta), \quad F^{\omega_s} = F^{\omega_s}(\zeta, \sigma_{eq}^c, \omega, \Theta), \quad F^{\omega_t} = F^{\omega_t}(\zeta, \sigma_{eq}^c, \sigma_{eq}^{\omega_t}, \omega, \Theta)$$

$$\dot{\omega} = \Psi(\omega, \sigma_{eq}^{\omega_s}, \sigma_{eq}^{\omega_t}, \Theta), \quad \dot{\zeta} = Z(\zeta, \sigma_{eq}^c, \omega, \Theta)$$

where $\dot{\varepsilon}_s$, F, F^{ω_s}, F^{ω_t}, $\dot{\omega}$, ζ, denote steady-state rate-of-deformation, the transient function for dislocation creep, the transient function for shear-induced damage, the transient function for tensile-induced damage, the damage evolution equation and the strain-hardening evolution equation, respectively; I_1, is the first invariant of Cauchy stress; T_1, and T_3 are the maximum and minimum principal Cauchy stresses respectively; and Θ is absolute temperature.

THERMODYNAMIC CONSISTENCY

The MDCF model is formulated in terms of conjugate pairs for which a sum of products gives the rate of stress-work per unit volume. It has been shown (Fossum *et al.* [1988]) that the rate of entropy production per unit volume, in terms of total and reversible stress work per unit volume, from dissipation is

$$\dot{\delta} = \frac{\dot{W} - \dot{W}^R}{\Theta} = \frac{\sigma_{eq}^i \dot{\varepsilon}_{eq}^i}{\Theta} \quad (3)$$

Since this quantity must be non-negative for a closed system,

$$\dot{W}^I = \sigma_{eq}^i \dot{\varepsilon}_{eq}^i \geq 0 \quad (4)$$

where $\dot{W}^I$ denotes the rate of increase of inelastic stress work per unit volume. The MDCF expressions for $\sigma_{eq}^i \dot{\varepsilon}_{eq}^i$ satisfy Eq. (4) and thus the MDCF equations do not violate the laws of thermodynamics.

COORDINATE INVARIANCE

There is an importance difference between coordinate invariance and frame indifference; it is not necessary to define a frame with a coordinate system. Coordinate invariance will be satisfied if the physical quantities in constitutive equations are described directly as scalars, vectors, or tensors without reference to coordinate systems. For example, the equivalent stress measures of the MDCF equations are written in terms of Cauchy principal stresses and the first Cauchy stress invariant without reference to a specific coordinate system. Because of this and because the kinetic equations of the MDCF equations are written in terms of coordinate invariant scalars and scalar functions of invariants, the MDCF equations are coordinate invariant.

FRAME INDIFFERENCE

Frame indifference implies that a quantity is invariant under all changes of frame defined by the following (Truesdell [1965]):

$$x^* = c(t) + Q(t)(x - x_0), \quad t^* = t - a \qquad (5)$$

where $c(t)$ represents a time-dependent point; $Q(t)$ is a time-dependent orthogonal transformation; x_0 is a fixed point; and a is a constant. The *principle of material indifference* (PMI) (Truesdell & Noll [1965]) states that for reference frames $(0^*, x^*)$ and $(0, x)$ defined through Eq. (5), the stress tensors T^* and T are related by $T^* = QTQ^t$ and the constitutive equation is invariant. The PMI says that indifferent quantities, except for a rotation, are independent of the reference frame. Indifferent scalars and vectors transform respectively as $f^* = f, \quad v^* = Qv$. The material time derivative of the Cauchy stress tensor is given by

$$\dot{T}^* = Q\dot{T}Q^t + \dot{Q}TQ^t + QT\dot{Q}^t \qquad (6)$$

and thus is *not* frame indifferent because of the existence of the second and third terms on the right-hand side of Eq. (6). For this reason, a different time derivative, called the Green-Naghdi stress rate, $\hat{\sigma}$, is used in the MDCF equations. The Green-Naghdi stress rate is given by

$$\hat{\sigma} = \dot{T} - \dot{R}R^t T + T\dot{R}R^t \qquad (7)$$

in which R is the rotational component tensor of the deformation gradient, $F = RU$ where U is the positive definite and symmetric right stretch tensor. The Green-Naghdi rate of Cauchy stress can be envisioned to evolve as follows. First, the Cauchy stress, T, is de-rotated with a proper orthogonal rotation tensor, R, from the current configuration to an intermediate configuration, $\underline{T} = R^t TR$. Then a material time derivative is taken of the de-rotated Cauchy stress, i.e.,

$$\dot{\underline{T}} = R^t\dot{T}R + \dot{R}^t TR + R^t T\dot{R} \qquad (8)$$

The rate of de-rotated Cauchy stress is then rotated back to the current configuration, $\hat{\sigma} = R\dot{\underline{T}}R^t$. Note that in the absence of rigid-body rotations, the Green-Naghdi stress rate reduces to the Cauchy stress rate.

The Green-Naghdi stress rate can be shown to be frame indifferent as follows. It is required by the PMI that $\hat{\sigma}^* = Q\hat{\sigma}Q^t$. By using the fact that $R^* = QR$ (Truesdell [1965]), from which it follows that $\dot{R}^* = \dot{Q}R + Q\dot{R}$, we find

$$\begin{aligned}
\hat{\sigma}^* &= \dot{T}^* - \dot{R}^* R^{t*} T^* + T^* \dot{R}^* R^{t*} = Q\dot{T}Q^t + \dot{Q}TQ^t + QT\dot{Q}^t \\
&\quad - (\dot{Q}R + Q\dot{R})R^t Q^t QTQ^t + QTQ^t(\dot{Q}R + Q\dot{R})R^t Q^t \\
&= Q(\dot{T} - \dot{R}R^t T + T\dot{R}R^t)Q^t = Q\hat{\sigma}Q^t
\end{aligned} \qquad (9)$$

thereby showing that $\hat{\sigma}^* = Q\hat{\sigma}Q^t$ is recovered, and hence the Green-Naghdi stress rates are frame indifferent.

The MDCF equations take the functional form $\hat{\sigma} = f(D - D^I)$ and the PMI requires that $\hat{\sigma}^* = f(D^* - D^{I*}) = Qf(D - D^I)Q^t = Q\hat{\sigma}Q^t$. The rate-of-deformation tensor, D, is frame indifferent (Truesdell [1965]) and so $D^* = QDQ^t$. The inelastic rate-of-deformation tensor, D^I, given by Eq. (1), comprises the sum of products of kinetic functions and Cauchy stress derivatives of conjugate equivalent stress measures for each of the mechanisms. Kinetic functions are scalar-valued tensor functions and are invariants since their forms as functions of components are the same for all bases related by orthogonal transformations. Thus, $\dot{\varepsilon}_{eq}^{i*} = \dot{\varepsilon}_{eq}^{i}$ ($i = c$, ω_s, ω_t). By the same reasoning, each of the conjugate equivalent stress measures is an invariant. As invariant scalar-valued tensor functions, the conjugate equivalent stress measures are isotropic and

$$\sigma_{eq}^{i*}(T) = \sigma_{eq}^i(T) = \sigma_{eq}^i(QTQ^t) \quad (i = c,\ \omega_s,\ \omega_t) \tag{10}$$

The stress derivatives of the invariants, $\sigma_{eq}^i(T)$, are consequently isotropic tensor-valued tensor functions (Truesdell & Noll [1965]) and

$$\frac{\partial \sigma_{eq}^{i*}}{\partial T} = \frac{\partial \sigma_{eq}^i}{\partial T}(QTQ^t) = Q\frac{\partial \sigma_{eq}^i}{\partial T}(T)Q^t \quad (i = c,\ \omega_s,\ \omega_t) \tag{11}$$

From Eqs. (1), (11), and the fact that $\dot{\varepsilon}_{eq}^{i*} = \dot{\varepsilon}_{eq}^{i}$ ($i = c$, ω_s, ω_t) we find

$$D^{I*} = \frac{\partial \sigma_{eq}^{i*}}{\partial T}\dot{\varepsilon}_{eq}^{i*} = Q\frac{\partial \sigma_{eq}^i}{\partial T}\dot{\varepsilon}_{eq}^i Q^t = QD^IQ^t \quad (i = c,\ \omega_s,\ \omega_t) \tag{12}$$

Thus, we see that $f[D^* - D^{I*}] = f[Q(D - D^I)Q^t]$. It follows that the PMI requires f to be an isotropic tensor-valued function of the tensor, $D - D^I$, such that

$$Qf(D - D^I)Q^t = f[Q(D - D^I)Q^t] \tag{13}$$

A representation of an isotropic tensor-valued function (Truesdell & Noll [1965]) can then be used to define the algebraic form of f, as

$$f(D - D^I) = \phi_0 I + \phi_1(D - D^I) + \phi_2(D - D^I)^2 \tag{14}$$

where I is the unit tensor. If we now choose

$$\phi_0 = \lambda tr(D - D^I), \ \phi_1 = 2\mu, \ \phi_2 = 0 \tag{15}$$

where λ and μ are Lame's constants and tr denotes the trace, we recover the frame indifferent MDCF equations,

$$\hat{\sigma} = \lambda tr(D - D^I)I + 2\mu(D - D^I) \tag{16}$$

We have chosen a linear form of Eq. (14) since the difference, $D - D^*$, is expected to be small, representing elastic lattice strain.

PHYSICAL ADMISSIBILITY

A constitutive equation is said to be physically admissible if the dependence of deformation and rate-of-deformation at time t on the stress or stress-

temperature history in the interval $0 \leq t$ is continuous. This means that given two stress-temperature histories $T(\tau)$, $\Theta(\tau)$ and $T^*(\tau)$, $\Theta^*(\tau)$ the following must be true,

$$|E^* - E| \to 0, \quad \|T^* - T\| \to 0, \quad \|\Theta^* - \Theta\| \to 0 \qquad (17)$$

where E denotes some inelastic strain measure such as Green strain and the double vertical lines denote a supremum norm, i.e., the greatest value of the argument for some τ lying in the interval $0 \leq t$. In the limit, the difference between the two stress-temperature histories becomes negligible. Yet, if the strains were not continuous at time τ they would depend upon which of the two stress-temperature histories were used to describe the load path.

Let two nearby stress-temperature histories be denoted by T, Θ and $T + \Delta T$, $\Theta + \Delta \Theta$ in the time interval $0 \leq t_1$. Correspondingly, ζ, σ_{eq}^c, $\sigma_{eq}^{\omega_s}$, $\sigma_{eq}^{\omega_t}$, ω and $\zeta + \Delta \zeta$, $\sigma_{eq}^c + \Delta \sigma_{eq}^c$, $\sigma_{eq}^{\omega_s} + \Delta \sigma_{eq}^{\omega_s}$, $\sigma_{eq}^{\omega_t} + \Delta \sigma_{eq}^{\omega_t}$, $\omega + \Delta \omega$ are defined.

Let the initial conditions for $\Delta \zeta$, ΔT, $\Delta \omega$, $\Delta \Theta$ be zero when $t = 0$. It follows immediately that $\Delta \sigma_{eq}^c$, $\Delta \sigma_{eq}^{\omega_s}$, $\Delta \sigma_{eq}^{\omega_t} = 0$ when $t = 0$. The evolution equations, from Eq. set (2), then become

$$\Delta \dot{\zeta} = \frac{\partial Z}{\partial \zeta} \Delta \zeta + \frac{\partial Z}{\partial \sigma_{eq}^c} \Delta \sigma_{eq}^c + \frac{\partial Z}{\partial \omega} \Delta \omega + \frac{\partial Z}{\partial \Theta} \Delta \Theta \qquad (18)$$

$$\Delta \dot{\omega} = \frac{\partial \Psi}{\partial \omega} \Delta \omega + \frac{\partial \Psi}{\partial \sigma_{eq}^{\omega_s}} \Delta \sigma_{eq}^{\omega_s} + \frac{\partial \Psi}{\partial \sigma_{eq}^{\omega_t}} \Delta \sigma_{eq}^{\omega_t} + \frac{\partial \Psi}{\partial \Theta} \Delta \Theta \qquad (19)$$

Now if we specify T and Θ as functions of time, then σ_{eq}^c, $\sigma_{eq}^{\omega_s}$, $\sigma_{eq}^{\omega_t}$ are known functions of time and consequently ω and ζ are known functions of time through integration. Then, if we specify $\Delta \Theta$ and ΔT as functions of time, $\Delta \sigma_{eq}^c$, $\Delta \sigma_{eq}^{\omega_s}$, $\Delta \sigma_{eq}^{\omega_t}$ will also be known functions of time. Moreover, the second and third terms on the right-hand side of Eq. (19) become known functions of time. Thus, Eq. (19) can be integrated to determine $\Delta \omega$ with initial condition $\Delta \omega = 0$ at $t = 0$. Now, with $\Delta \omega$ known, the second, third, and fourth terms of Eq. (18) are known functions of time. Thus, Eq. (18) can be integrated to determine $\Delta \zeta$ with initial condition $\Delta \zeta = 0$ at $t = 0$. The solutions to Eqs. (18) and (19) become

$$\Delta \zeta(t) = \exp\left(\int_0^t \frac{\partial Z}{\partial \zeta} d\tau\right) \int_0^t \left\{ \left[\frac{\partial Z}{\partial \sigma_{eq}^c} \Delta \sigma_{eq}^c + \frac{\partial Z}{\partial \omega} \Delta \omega + \frac{\partial Z}{\partial \Theta} \Delta \Theta \right] \exp\left(-\int_0^\tau \frac{\partial Z}{\partial \zeta} d\zeta\right) \right\} d\tau \qquad (20)$$

$$\Delta \omega(t) = \exp\left(\int_0^t \frac{\partial \Psi}{\partial \omega} d\tau\right) \int_0^t \left\{ \left[\frac{\partial \Psi}{\partial \sigma_{eq}^{\omega_s}} \Delta \sigma_{eq}^{\omega_s} + \frac{\partial \Psi}{\partial \sigma_{eq}^{\omega_t}} \Delta \sigma_{eq}^{\omega_t} + \frac{\partial \Psi}{\partial \Theta} \Delta \Theta \right] \exp\left(-\int_0^\tau \frac{\partial \Psi}{\partial \omega} d\zeta\right) \right\} d\tau \qquad (21)$$