FORMULATION OF A BONDED-PARTICLE MODEL TO SIMULATE STRESS CORROSION IN ROCK

D.O. Potyondy
Department of Civil Engineering and Lassonde Institute, University of Toronto, Canada

ABSTRACT

The bonded-particle model for rock (BPM, Potyondy and Cundall [1]) is enhanced to include time-dependent behavior. The BPM represents rock by a dense packing of non-uniform-sized circular or spherical particles that are bonded together at their contact points and whose mechanical behavior is simulated by the distinct-element method. Damage is represented explicitly as broken bonds, which form and coalesce into macroscopic fractures when load is applied. This system mimics a cemented granular material of complex-shaped grains in which both the grains and the cement are deformable and may break, and thus exhibits a rich set of emergent behaviors that correspond very well with those of real rock. The enhanced model is called the Parallel-bonded Stress Corrosion model (PSC model, Potyondy [2]), because it mimics the stress-dependent corrosion reaction that occurs in silicate rocks in the presence of water. Force transmission through rock, and through a BPM, produces many sites of micro-tension, and it is postulated that stress-corrosion reactions may be occurring at these sites. The stress-corrosion process is implemented in the PSC model by removing bonding material at a specified rate at each parallel bond that is loaded above its micro-activation stress, and chemical reaction rate theory is used to obtain a reasonable parameterization and stress dependence of the corrosive-front velocity — see Figure 1. Global force redistribution occurs throughout the process, and parallel bonds are removed from the system either by breakage (when their strength is exceeded) or by complete bond dissolution (when $\bar{D} \to 0$). The three PSC model parameters can be chosen to match both the static-fatigue curve (time-to-failure versus applied load) and the damage mechanisms and deformation behavior (a creep curve showing primary, secondary and tertiary creep) of Lac du Bonnet granite. The PSC model provides a consistent description of subcritical crack growth in rock that embraces both the microscopic processes of reactions and thermal activation at crack tips and the more mesoscopic processes of microcrack-microstructure-macrocrack interaction. The fact that the PSC model bypasses the need to idealize the rock in the classical Linear Elastic Fracture Mechanics (LEFM) sense, yet can itself reproduce LEFM behavior, suggests that it may be a more general model of rock that more closely mimics the physical behavior mechanisms than does an LEFM material.
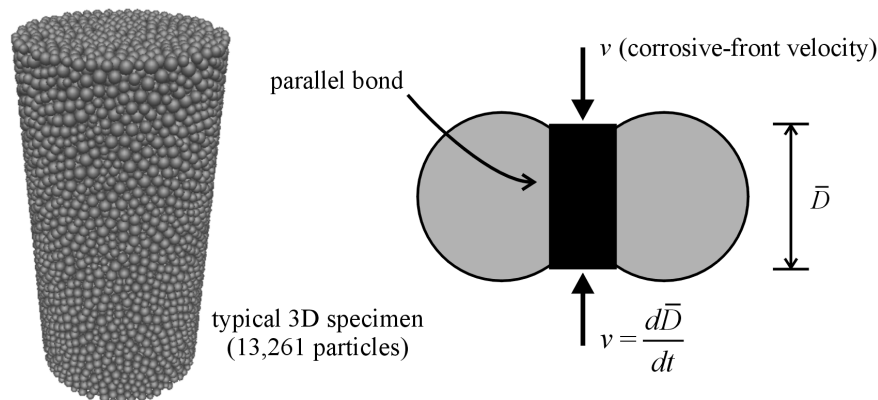
Figure 1: Primary mechanism implemented in the PSC model (v is a function of the maximum tensile stress acting on the bond periphery).

1 INTRODUCTION

Time-dependent weakening processes aided by water and other fluids occur in rock. These processes are reviewed by Kirby and McCormick [3], and the following summary focusing on rock behavior in the brittle regime (herein defined as the pressure interval over which extension and shear fracturing and faulting occur) is taken from their review.

The effects of the time scale of load duration generally are revealed by the effects of strain rate on strength in constant strain rate tests and by the variation of strain rate with time at constant differential stress in creep tests. Fundamentally, these time-dependent effects stem from the aid that thermal vibrations of atoms provide to deformation processes: the longer the duration of load, the greater the probability that a thermal vibration of sufficient amplitude to aid the deformation process will occur. The time-dependent behavior of rock in the brittle regime depends strongly on the initial porosity with pore collapse and microcracking each contributing. Low-porosity crystalline rocks exhibit a static-fatigue response. Creep strains are produced by microcracking involving the extension of preexisting cracks and the production of new cracks.

The mechanism responsible for the time dependence of brittle creep is thought to be corrosion of crack tips by chemical hydration (stress corrosion), and creep rates are thought to be controlled by the rate of slow growth of tensile cracks. At low strains, tensile cracks extend from stress concentrators (cracks, pores, grain boundaries, etc.), and the rates of growth decrease as the number of concentrators is exhausted by cracking, and thus creep rates decrease with increasing time in the hardening stage. If the crack density exceeds some critical value such that cracks are close enough to interact on a large scale, crack coalescence occurs to form a macroscopic fracture on which failure occurs.

The PSC model mimics the time-dependent weakening process of stress corrosion. The associated damage interactions that lead to macroscopic fracture formation are emergent properties of this model that arise from its implementation within a bonded-particle model for rock.

2 FORMULATION

Assume that time-dependent behavior of silicate rock in the brittle regime is controlled by a stress corrosion reaction (in which water attacks the Si-O bonds of the material in regions experiencing large stress-induced volumetric expansion), and that this reaction can be represented using reaction rate theory (Masel [4]) for which the reaction kinetics are embodied in the chemical reaction-rate equation (Lockner [5]):

$$\ln\left(\frac{r}{r_o}\right) = c - \left(\frac{E^* - v^* \sigma_{rs}}{RT}\right) \qquad (1)$$

where r is reaction rate, r_o and c are constants, R is the gas constant, T is the absolute temperature, σ_{rs} is the reaction site stress, and E^* and v^* are apparent activation energy and activation volume, respectively. Equation (1) states that an energetically favored reaction will progress at a rate determined by the rate of successful attempts to overcome an energy barrier represented by the activation energy. In addition, if the reaction sites are stressed, the effective energy barrier is reduced by an amount $v^* \sigma_{rs}$.

The reaction site stress, σ_{rs}, is difficult to quantify. Most workers have idealized the system as an isotropic linear elastic material containing large cracks, measured crack growth rate, and related it to the stress intensity factor, K_I, at the crack tip. This will be referred to as the LEFM assumption. Freiman [6] derives a model for stress-assisted crack propagation in glasses and ceramics based on a molecular model of stress-induced chemical reaction between vitreous silica

and water (Michalske and Freiman [7]). The model considers the materials to be ideally brittle (i.e., there are no zones of plastic deformation at propagating crack tips), and thus, fracture is governed by bond-breaking mechanisms. The model is based on the premise that highly concentrated tensile stress fields exist at a crack tip. Continuum approximations indicate that the bridging Si-O bond experiences strains > 20%. The effect of this strain on the bonding molecular orbitals is not easy to predict but can be discussed in terms of a decrease in the overlap between atomic orbitals, thus increasing their availability for bonding with other species. Freiman's model assumes that crack velocity is directly proportional to reaction rate, and provides a theoretical basis for expressing crack velocity in the form $V = V_0 \exp(bK_I)$ by assuming that the tensile stress dependence of the reaction rate can be expressed as the negative of the pressure dependence such that the term $v^*\sigma_{rs}$ in eqn. (1) is replaced by the term bK_I, where $b = v^*(\pi d)^{-1/2}$ and d depends on the structure of the crack tip. We use eqn. (1) to describe the reaction kinetics, and only set $v^*\sigma_{rs} = bK_I$ when employing the LEFM assumption.

The BPM does not employ the LEFM assumption; instead, it mimics the mechanical behavior of a collection of grains joined by cement. In the following discussion, we consider each grain as a BPM particle and each cement entity as a parallel bond. Equation (1) is applied to the BPM by making the following assumptions.

(a) The stress-corrosion reaction only affects the cement, it does not affect the grains; therefore, each parallel bond is a potential reaction site.

(b) The reaction occurs at the bond surface, and removes bond material at a uniform rate that is proportional to the reaction rate in eqn. (1). The rate of material removal is called the corrosion rate. We can envision the removal process as an edge crack growing uniformly into the bond material along its periphery.

(c) The corrosion rate is dependent on the stress at the reaction boundary, and this stress is taken as the maximum tensile stress acting on the bond periphery.

(d) Corrosion only occurs when the local driving stress is tensile and above some threshold level.

We express the corrosion rate as the rate at which the parallel-bond diameter, $\bar{D}$, decreases by (assumptions (a) and (b)):

$$\frac{d\bar{D}}{dt} = -\alpha r = -\left(\alpha r_o e^c e^{-E^*/RT}\right)e^{v^*\sigma_{rs}/RT} \qquad (2)$$

where α is the constant of proportionality between the corrosion rate and the reaction rate. The reaction site stress is related to $\bar{\sigma}$, the maximum tensile stress acting on the parallel bond periphery (assumption (c) above), and it is assumed that there is a threshold stress, $\bar{\sigma}_a$, below which the stress-corrosion reaction ceases (assumption (d) above), so that eqn. (2) can be expressed as

$$\frac{d\bar{D}}{dt} = \begin{cases} -\beta_1 e^{\beta_2(\bar{\sigma}/\bar{\sigma}_c)}, & \bar{\sigma} \geq \bar{\sigma}_a \\ 0, & \bar{\sigma} < \bar{\sigma}_a \end{cases} \qquad (3)$$

where $\bar{\sigma}$ has been normalized by the parallel-bond tensile strength $\bar{\sigma}_c$. The PSC model is described in eqn. (3) by the rate at which the diameter, $\bar{D}$, of each parallel bond decreases. The variables are the maximum tensile stress acting on the bond periphery ($\bar{\sigma}$) and the elapsed time since bond formation (t). The parameters are the two rate constants (β_1, with units of velocity and the dimensionless constant β_2), the micro-activation stress ($\bar{\sigma}_a$) and the parallel-bond tensile strength ($\bar{\sigma}_c$). The two rate constants are related to the reaction-rate parameters in eqn. (1) by

$$\beta_1 = \alpha r_o e^c \exp\left(-E^*/RT\right)$$

$$\beta_2 = \left(\frac{\bar{\sigma}_c}{\bar{\sigma}}\right)\left(\frac{v^* \sigma_{rs}}{RT}\right). \tag{4}$$

3 IMPLEMENTATION

The PSC model introduces a time-dependent behavior into the BPM, thereby making it necessary to simulate the advancement of time in order to reduce the parallel-bond diameters by integrating eqn. (3). Two separate accumulated times are maintained, one for the particle assembly and another for the stress-corrosion model. During a stress-corrosion simulation, the BPM provides the force and moment distributions corresponding with a series of static-equilibrium states between which the parallel-bond diameters are reduced. If the BPM is run with high numerical damping, then quasi-static conditions are approximated at all times; however, if the BPM is run with low numerical damping, then seismic source information can be obtained during the cracking episodes (Hazzard and Young [8]) that occur during the force-redistribution following the parallel-bond diameter reductions.

The following three-step procedure allows one to simulate the time evolution of a particle assembly undergoing stress corrosion. The simulation proceeds until either (1) the desired stress-corrosion time is reached, (2) the system fails (i.e., a static-equilibrium state cannot be obtained for the current loading) or (3) the maximum tensile stresses acting on the periphery of all parallel bonds are below the respective micro-activation stresses indicating that, for the current loading, no further stress-corrosion damage will occur.

1. Cycle the BPM until a state of static equilibrium has been obtained. Equilibrium is determined based on the user-specified equilibrium ratio limit, f_r, expressed as the ratio of maximum unbalanced force magnitude over all particles divided by average applied force magnitude over all particles. After each increment of stress-corrosion time, the model is cycled until this ratio falls below f_r.
2. For a given stress-corrosion timestep, reduce the diameters of all parallel bonds by integrating eqn. (3).
3. Return to step 1.

While stress corrosion is active, there are two means by which parallel bonds are removed from the system. Either the bond tensile ($\bar{\sigma}_c$) or shear ($\bar{\tau}_c$) strength is exceeded causing the bond to break, or the bond diameter falls below a minimum allowable value (typically taken as 1% of the original bond diameter). The bond-dissolution mechanism can occur when diameter reduction and subsequent force redistribution maintain the condition: $\bar{\sigma}_a \leq \bar{\sigma} < \bar{\sigma}_c$ and $\bar{\tau} < \bar{\tau}_c$. Such is the case for a two-particle system carrying a pure tensile load and subjected to fixed-displacement conditions. Such stable bond-dissolution processes also occur in synthetic specimens subjected to static-fatigue loading, suggesting a difference in the damage fabric that develops during long- and short-term loading conditions.

During a stress-corrosion simulation, the stress-corrosion timestep, Δt, can be kept constant at a specified value or chosen automatically using the following procedure, which varies Δt in response to system behavior such that the timestep decreases during periods of rapid damage accumulation and increases during periods of relative quiescence. This self-adaptive procedure is necessary to simulate most systems within a reasonable number of steps. The elapsed time to the first parallel bond failure, t_f, is estimated by assuming that parallel-bond forces and moments are constant during the increment. The timestep is taken as

$$\Delta t = \left(1/n_s\right)t_f \tag{5}$$

where n_s is the number of steps until the first parallel bond breaks (assuming a perfect estimate). We define a subinterval as the sequence of timesteps that occur from the time of estimation until the first parallel bond actually breaks. The subinterval ends when at least one parallel bond has broken. A new estimate using eqn. (5) is made at the start of each subinterval. To prevent large numbers of small steps being taken during a subinterval, the timestep is multiplied by a factor, f_s $\left(f_s > 1.0\right)$, after every n_s steps of the subinterval.

Both the accuracy and the execution speed of the stress-corrosion procedure are controlled by the algorithm-control parameters f_r, n_s and f_s. The best accuracy is obtained when $f_r \to 0$ and $\Delta t \to 0$. Typically f_r is set equal to a small value on the order of 10^{-5}, and the timestep is chosen automatically with $n_s = 2$ and $f_s = 2.0$. For particular boundary-value simulations, it is necessary to determine the effect of these algorithm-control parameters on system response. Both two- and three-dimensional static-fatigue simulations indicate that the size of the stress-corrosion timestep affects the macroscopic time to failure. As $\Delta t \to 0$, the true macroscopic time to failure is approached from above.

4 COMPARISON WITH LEFM-BASED MODELS

The PSC model is compared with LEFM-based models of subcritical crack growth as follows. The LEFM-based models (Kemeny [9]; Kemeny and Cook [10]; Lockner and Madden [11]; Okui and Horii [12,13]) postulate an initial collection of cracks, and then grow these cracks at a velocity that is a function of stress-intensity factor ($V = AK^n$, $K \geq K_{th}$), where K_{th} is the stress-corrosion threshold. The PSC model postulates an initial collection of grains joined by cement, and then removes the cement at a rate that is a function of local maximum tensile stress ($d\bar{D}/dt = -\beta_1 e^{\beta_2(\bar{\sigma}/\bar{\sigma}_c)}$, $\bar{\sigma} \geq \bar{\sigma}_a$), where $\bar{\sigma}_a$ is the stress-corrosion threshold. There are three levels of "cracks" in the PSC model. At the micro-level, a crack exists in each parallel bond as soon as its diameter begins to be reduced (see assumption (b) above), at the meso-level, a crack exists as a single broken or fully dissolved parallel bond, and at the macro-level, a crack exists as a contiguous collection of broken or fully dissolved bonds. As the length of such a macrocrack becomes large relative to the particle size, the conditions at its tip become well characterized by LEFM assumptions. In the LEFM-based models, the macrocrack velocity, V, is an indirect input parameter (based on A and n), whereas in the PSC model, the microcrack velocity (or corrosion rate) is an indirect input parameter (based on β_1 and β_2) and the macrocrack velocity is an emergent property. Potyondy and Cundall [1] demonstrate a formal equivalence between the mechanisms and parameters of the BPM and the concepts and equations of LEFM. These relations can be used to show that the macrocrack velocity of the PSC model can be expressed in the form $V = V_0 \exp\left(bK_I\right)$. This is the same form as Freiman's model, and thus, justifies the use of eqn. (3) to express the corrosion rate of each parallel bond.

5 CONCLUSIONS

The PSC model can be calibrated by matching 1) the time-to-failure curve produced by performing a series of static-fatigue tests, 2) the loading-rate dependence of compression strengths, or 3) the velocity versus stress-intensity factor curve of a single macroscopic fracture subjected to pure mode-I tension. The first calibration procedure has been performed for both the two- and three-dimensional models. During a static-fatigue test, the axial load and confinement

are held constant, and both the time-dependent deformation and possible time to failure are measured. The three PSC model parameters can be chosen to match the static-fatigue curve (time-to-failure versus applied load) for Lac du Bonnet granite. Also, the synthetic material exhibits damage mechanisms and deformation behavior that are similar to those of the rock. The response is characterized by a creep curve, whereby the axial strain increases with time, and the response can be divided into the three stages of primary, secondary and tertiary creep.

The PSC model could be used to better understand the time-dependent weakening processes that occur in rock by matching quantitatively the response of a specific rock undergoing the three loading regimes described above. Achieving such a match may require modification of eqn. (3) and a more realistic replication of the rock microstructure than has been done to date (predominantly only dense packings of near-uniform particle size distributions have been employed). Also, further insight may be gained by relating the macroscopic response to the thermodynamic quantities in eqn. (4). The PSC model is a comprehensive rock model that consistently combines processes occurring over a range of spatial and temporal scales. One application of such a model is to better understand the long-term damage processes that occur around an excavation (of say, a nuclear waste emplacement) to aid in the prediction of excavation stability and long-term strength for times up to and beyond 10,000 years.

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