FRACTURE ANALYSIS OF CEMENTITIOUS SEALS FOR NUCLEAR WASTE ISOLATION

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This paper presents the finite element analysis of cementitious seals for underground nuclear waste isolation by using an analysis approach which couples continuum microcracking damage mechanics, nonlinear fracture mechanics, and linear elastic fracture mechanics analyses through a new coupling method called "structural zooming". Also the continuum microcracking damage mechanics model originally developed by L. Costin for compressive stress regimes is modified to accomodate tensile regimes of stress by using an apparent fracture toughness concept. The crack-tip process zone length is defined and the modified damage model is used to calculate the characteristics of a crack-tip process zone. A simple nonlinear fracture analysis approach for cementitious materials, in which the process zone is collapsed into a surface, is proposed. The process zone properties are calculated from basic material properties such as grain size and gross elastic moduli of cementitious materials.

INTRODUCTION

Cementitious seals for underground nuclear waste isolation must be designed to prevent fluid flow for at least 10,000 years. Assuming the material in a grouted rock joint or borehole shrinks over time, the problem is to determine if cracking will occur, and ultimately, whether such cracking provides a path through which fluid can flow.

Both fracture mechanics and continuum damage mechanics have been applied to the analysis of cementitious materials (1,2,4,6). The former considers the fracture mechanisms in the macro-mechanics sense, while the latter accounts for the microstructural mechanisms of material deformation in a continuum sense only. Although certain successes have been obtained, there remains a transition gap between them, in which neither approach is very accurate or economical.

A microcrack continuum damage mechanics model has been used to study the crack-tip process zone characteristics. The process zone properties can be calculated from the damage model parameters, from which it is possible to determine what type of fracture mechanics is appropriate for engineering problems of varying size scale. Our analyses show what type of fracture mechanics should be used to solve engineering problems of various size scale associated with various cementitious materials.

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A MICRO-CRACKING DAMAGE MODEL

It is known that cementitious materials such as cement, mortar and concrete contain many randomly distributed pre-existing micro-cracks. As loaded these micro-cracks grow, nucleate and coalesce. The reduction of stiffness of material caused by the micro-cracking is defined as material damage (Yazdani and Schreyer (1)). In recent years many continuum damage models have been developed to study the mechanical behavior of microcracking materials.

The model used here was originally developed by Costin and Stone (2,3). This model includes the effects of nucleation, growth and coalescence of micro-cracks on the deformation of the materials. The model directly uses some more fundamental material parameters such as micro-crack spacing and size, which makes the model easy to understand and physically meaningful.

It has been reported that cracks shorter than a certain length the apparent fracture toughness decreases with decreasing crack length (Ingraffea et al (4)). In the original Costin model the fracture toughness of the micro-cracks is taken as a constant. In the modified model, the apparent fracture toughness concept is used. It assumes that within the small crack length range, from $a = 0$ to $a = a_c$ (the critical crack length at which the apparent fracture toughness becomes constant), the apparent fracture toughness K_Q varies from K_{Q0} to K_{IC} parabolically. Fig. 1 shows the uniaxial tensile stress-strain curve obtained from the modified model applied to a single finite element.

THE COUPLED ANALYSIS APPROACH

The formation and propagation of cracks in cementitious seals involves both micro- and macro-cracking mechanisms. To model the entire process efficiently, both continuum damage mechanics and fracture mechanics analyses should be used and a special coupled analysis approach is needed. This can be accomplished through a new coupling method called "structural zooming" (Panthaki and Gerstle (5)), which makes it possible to couple a continuum damage mechanics finite element program with a linear elastic, mixed- mode, discrete crack propagation finite element program.

The proposed approach consists of three stages:

1. Global continuum damage mechanics analysis to determine the local region in which the maximum damage occurs due to the micro-cracking.
2. "Structural zooming" process to automatically transfer the boundary conditions obtained from the damage analysis to the local region, to refine the mesh in the local region and to introduce an initial macro-crack for the fracture mechanics analysis in the local region.
3. Linear elastic, mixed-mode, discrete crack propagation analysis to predict the crack propagation in the local region.

A sealing problem of a borehole in granite rock was analyzed by using the above approach. Assuming there is good compatibility on the grout/rock interface, the problem can be idealized as a circular region under plane strain condition subjected to a uniform outward radial displacement. Fig. 2 shows a small portion of finite element mesh in the local region with the introduced discrete crack after several steps of crack propagation analysis.

PREDICTION OF PROCESS ZONE CHARACTERISTICS

In recent years, many attempts have been made to predict and measure the characteristics of the crack-tip process zone in cementitious materials. It is found that up to now there is not a definitive definition for the process zone, which makes it very difficult to compare and use the data given in the literature.

Here we define the crack-tip process zone (assumed collapsed into a surface) as shown in Fig. 3. The process zone is assumed to start from the point where the stress σ is equal to 10% of the tensile strength σ_{max} and ends at the point where the crack opening displacement (COD), discussed below, vanishes.

As discussed before, since continuum damage mechanics can take into account the effects of microstructural changes on the material deformations it is reasonable to use it as a numerical experimental tool to predict the characteristics of the crack-tip process zone. Based upon the definition of crack-tip process zone discussed above, the modified Costin damage model was used to calculate the distributions of the stress and COD in the process zone and to predict the length of the process zone.

A rectangular panel with a central crack subjected to uniformly distributed displacement was used to predict the process zone characteristics. A quarter of the symmetrical panel was modeled using 98 4-noded finite elements, as shown in Fig 4. The damage was localized in the elements adjacent to the crack plane, as shown in Fig. 5. The distribution of COD caused by material damage can be obtained approximately by using the nodal displacements of the damaged elements ahead of the crack tip with the elastic portion subtracted out as follows

$$COD = \Delta_{total} - \Delta_{elastic} = \Delta_{total} - \frac{\sigma_a}{E} s \qquad \text{...(1)}$$

where the Δ's are nodal displacements normal to the crack surface, E is Young's modulus, σ_a is the average stress in the element and s is the width of the element normal to the crack surface. It is evident that the obtained COD is not objective with respect to the element width. According to some experimental observations (Petersson (6)), the process zone widths of concrete or similar materials are approximately equal to the maximum aggregate size. So it is reasonable to use elements with approximately this width to model the process zone. In the damage model used here the micro-crack spacing parameter d_l (3) is related to aggregate size (usually several aggregate sizes), so in the analysis elements with width equal to d_l were used. The Young's modulus, Poisson's ratio, d_l and K_{Ic} were assumed to be 2.2E4 MPa, .21, 0.004 m and 1.9 MPa-$m^{1/2}$, respectively.

The calculated stress-r and COD-r curves are shown in Fig. 6 and stress-COD curve is given in Fig. 7, with r is measured from the beginning of the process zone as defined in Fig. 3.

DISCUSSION

With the borehole sealing problem as an example, this paper has shown that it is possible to model the entire transition process of micro- to macro-cracking by coupling continuum damage mechanics and fracture mechanics analyses. In the analysis a uniform initial micro-crack distribution was assumed. The damage mechanics analysis was coupled with linear elastic fracture analysis. It would be more reasonable to couple a nonlinear fracture analysis approach (based upon a stress-COD curve, as shown in Fig. 7) with damage analysis, since at the beginning of macro-cracking the macro-crack initiated from the localized damage is still small compared with the process zone size.

Fig. 5 shows that the process zone produced by the model is localized into a narrow band with a length of approximately .025 m. It should pointed out that the process zone length predicted here is based upon the definition given in Fig. 3. If process zone is defined differently, say assuming it starts from the point where $\sigma = .05\sigma_{max}$, the predicted length will be longer. Also, this analysis shows that for relatively small cracks in cementitious materials, the crack-tip nonlinearity can not be neglected. By using continuum damage mechanics model to study the process zone characteristics, it is possible to establish a size thresholds beyond which nonlinear and linear elastic fracture analysis approaches should be used, which will be valuable for engineering analysis.

Based upon the prediction, a nonlinear fracture model for crack propagation analysis of cementitious materials is proposed here. Since the process zone is a very narrow band, it is very suitable to model the process zone by using interface elements with proper stress-COD curves programed in such that the feature of stress distribution as shown in Fig. 6 can reflected. From Fig. 7 it can be seen that a bilinear stress-COD curve may be used. The model will considerably simplify the analysis, since the crack-tip nonlinearity will be reflected only in the interface elements and the remeshing process can also be simplified. This model can be used in the coupled approach as discussed above. For further simplification, a linear elastic finite element analysis can be performed first and by identifying the region where the maximum tensile principal stress occurs interface elements can be inserted into the mesh in the direction perpendicular to the maximum tensile stress direction; then the propagation analysis can be performed.

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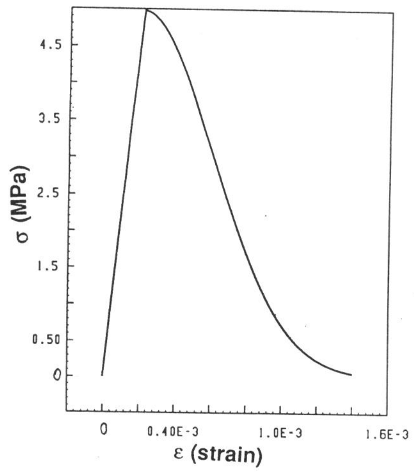

Figure 1 Uniaxial tensile stress-strain curve predicted by the modified microcracking damage model for one finite element.

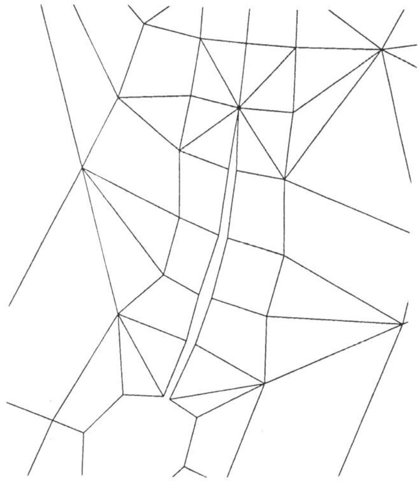

Figure 2 Discrete finite element crack propagation, using quarter-point singular elements, in the region local to a void.

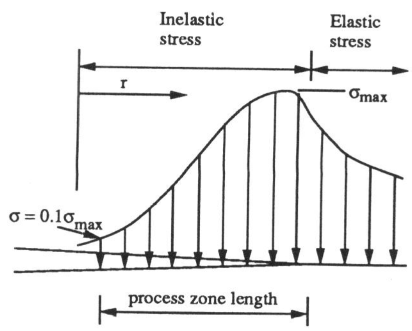

Figure 3 Sketch of crack-tip process zone with associated terminology. (Process zone is assumed to be collapsed into a surface.)

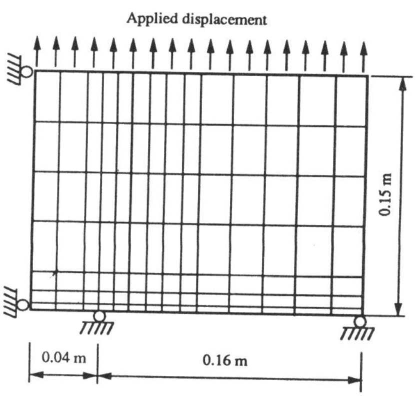

Figure 4 Finite element mesh used for prediction of process zone characteristics. (4-noded bilinear elements)

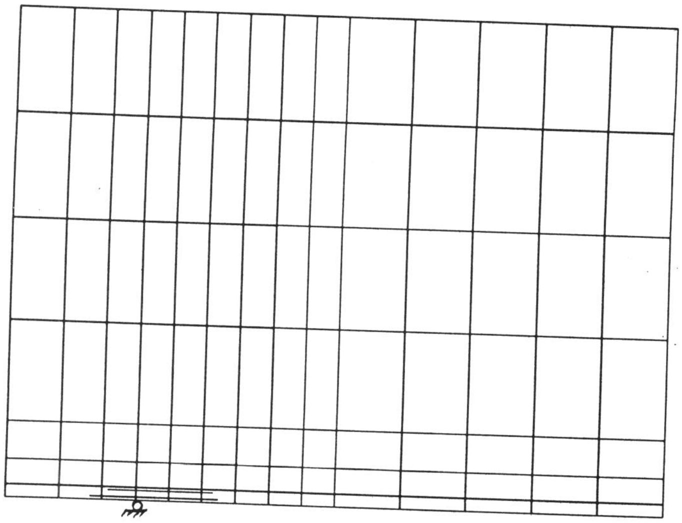

Figure 5 Damage vectors calculated from micro-cracking continuum damage finite element analysis predict that crack tip process zone is long and narrow.

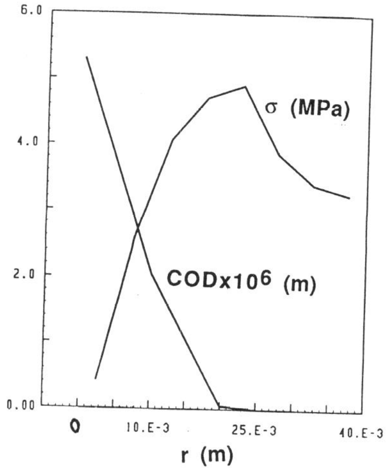

Figure 6 Stress versus r and COD versus r predicted by continuum microcracking damage model; mesh shown in Fig. 4.

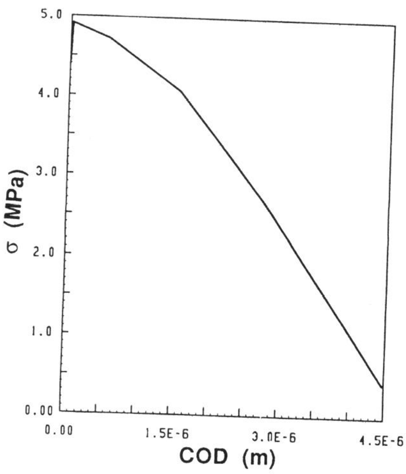

Figure 7 Stress-COD curve predicted by continuum microcracking damage model; mesh shown in Fig. 4.