Smeared와 Discrete 균열에 의한 암염의 유한요소해석

Finite Element Analysis of Combined Smeared and Discrete Mechanisms for Rock Salt

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요 약

지하 방사성 폐기물 저장소의 오랜기간동안의 거동은 지반의 파괴와 변형에 영향과 암염의 비선형변형의 예측은 어려운 실정이다. 따라서 본 연구는 암염의 비선형파괴 메커니즘과 비선형 연속체거동의 유한요소모델을 개발하였다.

Abstract

The long term behavior of the Waste Isolation Pilot Plant(WIPP), a nuclear waste repository currently under construction near Carlsbad at New Mexico, depends upon the fracture and deformation behavior of bedded rock salt. Although many numerical analyses of the WIPP have been conducted, to our knowledge none have included the ability to simultaneously predict the effects of fracture and nonlinear deformation of the salt continuum. We are in the process of developing a finite element program to simulate the effects of nonlinear fracture mechanics and nonlinear continuum behavior of rock salt simultaneously.

1. INTRODUCTION

Essential technology for storing nuclear waste products in salt formations is being developed in the Waste Isolation Pilot Plant(WIPP) program. One of the reasons for choosing natural salt deposites as the host site was that the time-dependent closure of rock salt storage rooms was expected eventually to encapsulate the waste in an impermeable envelope of salt. It is now known that the salt contains roughly 1 to 3% brine, and that there is therefore the possibility that the waste metals will corrode

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이 논문에 대한 토론을 1996년 6월 31일까지 본 학회에 보내주시면 1996년 12월호에 그 결과를 게재하겠습니다.

as they contact the brine, causing as a by-prod uct hydrogen gas. This gas, at the lithostatic pressure of the repository, has the potential to occupy a volume of roughly four times the original volume of the waste barrels. Continuum nonlinear finite element method(FEM) models have indicated that gas pressures in the repository may exceed the lithostatic pressure of 14.8 MPa by 10 MPa or more. The salt cannot sustain high tensile stress, and therefore such high gas pressures cannot in reality exist. This high predicted pressure indicates the possibility that a large gas-driven hydrofracture will form. In fact, analytical calculations have shown that, using the assumptions of linear elastic fracture mechanics(LEFM), a horizontal penny-shaped fracture five kilometers in radius(with less than and mm maximum crack opening) is possible. To better analyze and design the WIPP, it is necessary to have the cap ability to predict fracture propagation in salt rock.

LEFM is the classical theory of fracture mechanics, introduced by Griffith[1](Griffith 1920) and essentially completed by Irwin[2]. LEFM has two basic assumptions : (1) The continuum surrounding the crack is linear and elastic(follows Hooke's Law) ; and (2) the fracture process zone(FPZ) is confined to a small regioncompared to other dimensions in the problem. It is questionable whether the assumptions of LEFM are applicable to a gas-driven hydrofracture in salt because both of the above assumptions may be violated.

Since the LEFM calculation almost certainly over-predicts the crack length, it is reasonable to model the gas-driven hydrofracture using some form of nonlinear fracture mechanics that takes into account the time-dependent relaxation of the salt continuum as well as the possibly large FPZ at the tip of the crack. A recent paper[3] has shown that, even if the continuum is linear elastic, the fracture toughness of the crack pressurized by a viscous fluid far beneath the ground surface may depend upon crack length, and therefore violate the assumptions of LEFM. It is with these motivating ideas that we set out to develop a finite element capability to model combined smeared and discrete mechanisms in rock salt.

2. FEM MODELING OF FRACTURE

There are two fundamental techniques for modeling fracture using the FEM : the "discrete crack" and the "smeared damage mechanics" approaches. In the discrete crack approach, first suggested in the early 1960's[4], the propagation of a single crack is modeled by changing the finite element mesh to represent the new surfaces created by the crack. In this approach, the crack is viewed as a geometrical entity. In the approach, the crack is viewed as a geometrical entity. In the smeared damage mechanics approach[5] the growth of a crack or of a cracked region is represented by modifying the constitutive relations in affected finite elements. In the smeared damage mechanics model, the crack is viewed as a material entity.

The discrete crack approach requires, as a part of the analysis algorithm, automatic remeshing to accomodate crack propagation. In the past, this task has been so daunting that few have attempted to model automatic discrete crack propagation. Nonetheless, using modern software techniques, several successful two-dimensional algorithms have been developed[6,7,8,9]. Automatic remeshing to model crack propagation in three dimensions remains an unsolved problem. To model situations where the FPZ is small compared to other problem

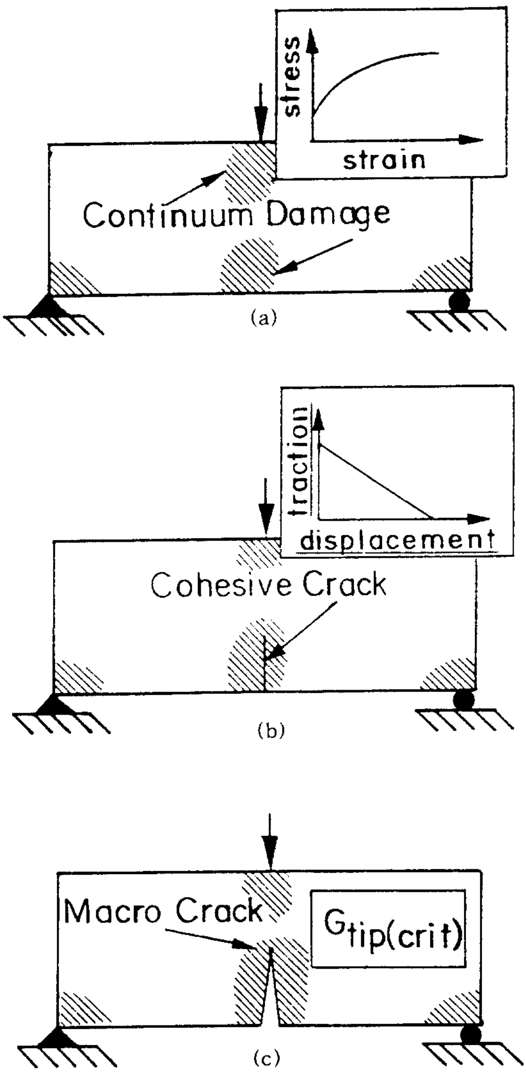

Fig.1 The complete development of a fracture includes
(a) continuum damage
(b) line-localization of damage at a "cohesive crack"
(c) development of a macro crack with damage localized at a point

dimensions as in LEFM the discrete approach is the only one that makes sense in terms of solution efficiency. Currently, two-dimensional discrete cracking implementations of LEFM analysis are becoming more common, while nonlinear fracture mechanics approaches using the fictitious crack model(also named the cohesive crack model) to model Dugdale-Barenblatt type cracks are beginning to appear in the literature.

The smeared damage mechanics approach is the only approach that makes sense when volumetrically distributed damage(say, in the form of stable micro crack growth) is to be modeled. However, it has been shown that the smeared damge mechanics approach fails to produce objective results with respect to mesh refinement when strain localization occurs[11)] Two principal schemes have been introduced to force the smeared damge mechanics approach to produce objective results with respect to mesh refinement : the "crack band model"[12)] and nonlocal damage mechanics[13)] The crack band model assumes that the FPZ is long and narrow(which is not always the case), and it fails when the element size becomes large compared to the FPZ length. On the other hand, the nonlocal damage models require the FPZ to be modeled explicitly, which is unreasonable when the FPZ becomes small compared to the size of the problem being analyzed. We propose, therefore, to incorporate features of both the discrete and the smeared damage mechanics models into a single FEM code. Relatively few large cracks will be modeled using the discrete crack approach (including the cohesive crack model), while volumetrically distributed mechanisms such as damage due to micro cracking, creep, and plasticity will be modeled using the smeared approach. An energy-based criterion will be developed, as described in the next section, to handle the transition from volume-dominated damage to surface-localized damage to point-localized damage, as suggested by Fig.1. To our knowledge, this approach has never before been suggested.

3. ENERGY APPROACH TO MODELING OF NON-LINEAR FRACTURE MECHANICS

The Griffith[1] criterion states that in a static problem, for a crack to propagate, the energy dissipated per unit crack propagation, G_f, must be equal to the potential energy release rate, G, which is the potential energy lost by the surrounding continuum per unit crack propagation :

$$G_f = G \tag{1}$$

In LEFM, G may be calculated from the stress intensity factors that characterize the stress field near the crack tip, and G_f is assumed to be a material constant.(It can in fact be proven that G_f must be a material constant.)

If we now make no assumptions about the constitutive relations that describe the behavior of the surrounding continuum, and also allow for a cohesive zone with nonlinear traction-displacement relations behind the crack tip, we can again state that the criterion for crack propagation is that the energy dissipation rate associated with the crack tip, G_{tip}, plus the energy dissipation rate associated with the cohesive zone, $G_{cohesive}$, plus the energy dissipation rate associated with the surrounding continuum, G_{volume}, must be equal to the rate of loss of potential energy in the problem :

$$G_{tip} + G_{cohesive} + G_{volume} = G, \tag{2}$$

or

$$G_{tip} = G - G_{cohesive} - G_{volume} \tag{3}$$

All of the terms in Eq.(3) can be calculated using standard finite element techniques except G_{tip}. This energy dissipation rate must be interpreted to be all that energy dissipated by the crack that is not explicitly accounted for by dissipation in the surrounding continuum, G_{volume}, or in the cohesive zone behind the crack tip, $G_{cohesion}$.

Now assume that the crack tip will propagate when G_{tip} reaches a critical value, $G_{tip(crit)}$, regardless of far-field conditions. There is a way to determine $G_{tip(crit)}$. We can solve the problem of a steady-state crack in an infinite medium. The energy dissipated by such a crack is the material property, G_f, which can be measured experimentally[14] or calculated. G_f is the sum of the energy dissipation rates :

$$G_f = G_{tip(crit)} + G_{cohesion} + G_{volume} \tag{4}$$

and therefore

$$G_{tip(crit)} = G_f - G_{cohesion} - G_{volume} \tag{5}$$

$G_{tip(crit)}$ is therefore interpreted as that portion of the energy dissipation rate associated with the crack tip that is not explicitly accounted for in the FEM model. Note that if no energy dissipation is included in the FEM model, then $G_{tip(crit)}=G_f$, and the problem reduces to a generalization of LEFM(with the difference being that the medium surrounding the crack may be nonlinear elastic).

The assumption that $G_{tip(crit)}$ is a material property is similar the assertion that G_f is a material property. We have essentially generalized our concept of fracture mechanics to include any level of explicit FPZ modeling, with the remainder of the energy dissipation rate assumed to be constant. $G_{tip(crit)}$ assumes the value of zero if the FPZ is modeled completely, and assumes the value of G_f if the FPZ is not modeled at all.

To use this approach effectively, it is necessary to choose the constitutive relations for the volume(stress-strain relations) and for the cohesive zone(traction-displacement relations) wisely, as indicated by the constitutive relations in Fig.1. Because the volumetrically smeared stress-strain constitutive models require special treatment only after achieving a zero eigenvalue(or a zero tangent stiffness), it makes sense to disallow negative eigenvalues in the stress-strain model. When the stress-strain relation develops a zero eigenvalue, then subsequently a cohesive crack is inserted at that location. Subsequent softening of the material is modeled by the cohesive crack model through an appropriate traction versus crack displacement constitutive relation.

At a given stage of crack development, in addition to determining whether a crack will propagate, it is necessary to determine in what direction it will propagate. Gerstle[15], to predict the direction of crack growth.

4. FEM IMPLEMENTATION

For several reasons it seems convenient to use linear triangular and bilinear quadrilateral elements to model combined smeared and discrete cracking. First, most nonlinear finite element codes are limited to simple linear and bilinear elements to avoid some of the spurious behaviors that may develop in higher order elements. Second, the automatic remeshing scheme to accommodate crack propagation is somewhat simpler for simple element types. Cohesive cracks may be modeled by linear displacement field interface elements[16]. We consider only infinitesimal displacements(small strains) currently, although in principle large displacements could be modeled as well. If large displacements were modeled, it would make more sense to use slide lines than interface elements to model the cohesive crack.

As explained in the previous section, under the proposed crack propagation criteria, it is necessary to determine the rates of energy dissipation with respect to crack length of both the continuum(G_{volume}) and the cohesive crack ($G_{cohesion}$), as well as the rate of change of potential energy(G).

The nonlinear finite element analysis capability must include continuum elements as well as interface elements. Gerstle et al have developed a nonlinear analysis code called NDFE(Nonlinear Dynamic Finite Element)[9]. NDFE has an explicit dynamic relaxation solver, a linear material model, and several simple nonlinear material models. Currently, no continuum model especially designed to model rock salt has been included, but we intend to add a salt model as soon as our testing, using simpler material models(linear elastic and local damage), is complete(See Fig.1(a)). NDFE also has a simple cohesive traction versus displacement model, as shown in Fig.1(b).

The solution procedure for static nonlinear crack propagation is as follows. In each time step, with the crack length held constant, iteration to an equilibrium solution is achieved. The dissipated energies $E_{volume}(a)$ and $E_{cohesion}(a$ and the potential energy E(a) are calculated by NDFE. Following this the crack length is incremented(by dragging the crack tip node) by a small amount, Δa. calculated to obtain $E_{volume}(a+\Delta a)$ and $E_{cohesion}(a+\Delta a)$ and the poten tial energy $E(a+\Delta a)$ at the incremented crack length. The energy release and dissipation rates are then approximated by the finite differences :

$$G = \frac{E(a+\Delta a) - E(a)}{\Delta a} \qquad (6)$$

$$G_{cohesion} = \frac{E_{cohesion}(a+\Delta a) - E_{cohesion}(a)}{\Delta a} \quad (7)$$

$$G_{volume} = \frac{E_{volume}(a+\Delta a) - E_{volume}(a)}{\Delta a} \quad (8)$$

Then Eq.(3) is employed to calculated G_{tip}. If G_{tip} is greater than or equal to $G_{tip(crit)}$ assumed a material constant, then the crack is incremented by the length of one finite element, using the automatic crack propagation remeshing program. The direction of crack propagation is calculated from the maximum circumferential tensile stress criterion[17]. Then the time is incremented and the process is repeated.

This approach can also be extended to accommodate dynamic crack propagation if the kinetic energy is included appropriately in the energy rate balance expressed by Eq.(2).

5. SIMPLIFIED REMESHING SCHEME

When a discrete crack propagates, the finite element mesh must be altered to model the geometrical change. We now consider only two-dimensional meshes ; automatic remeshing to accommodate crack propagation in three-dimensional problems is a much more complex problem, still to be solved. The crack propagation is an incremental process and at each step we make the assumption that the crack propagates across the next finite element in the path of the advancing crack. The crack remeshing algorithm consists in identifying all possible cases that can occur when a crack propagates in a FEM mesh with three-and four-noded elements and four-noded interface elements. Once identified, these cases can be programmed to make the crack propagation remeshing automatic. With a well-designed computational mechanics data base management system[18], this programming is easily accomplished. There are a limited number of cases(approximately 10) that need to be considered. Fig. 2 shows two of these cases : NSN and NE(4)S. Other cases, not shown, are NEN, NE(3)S, and DN(drag node). Fig.3 shows a mesh with a curved crack that has propagated through it using the algorithm. More detail on the remeshing algorithm is given in[15].

For three-dimensional problems the remesh-

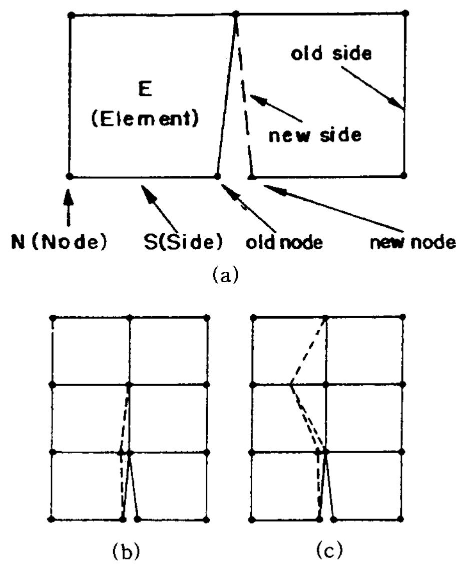

Fig.2 Schematic showing two cases in the automatic crack propagation remeshing algorithm. (a) symbols and abbreviations (b) case NSN : crack propagates from a node through a side to a node (c) case NE(4)S : crack propagates from a node through a four-noded element to a side.

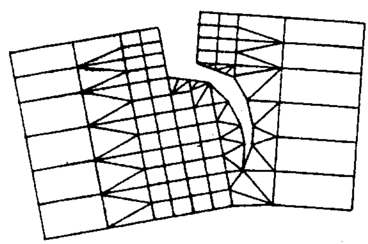

Fig.3 Mesh resulting from a curved crack propagating through a FEM mesh(6 propagation increments : deformed mesh shown).

ing to accommodate discrete crack propagation is much more complex. We believe that it might be easier to update the entire geometrical description of the algorithm to remesh the entire problem, rather than to attempt to modify the mesh locally, as we have done in the two-dimensional case.

6. CONVERGENCE CONSIDERATIONS

The FEM is an approximate method, and to be used effectively, the analyst must be aware of the accuracy of the analysis results. We have investigated the accuracy with which G_{tip} is calculated for meshes with varying degrees of concentrated upon the case of linear material behavior with G_{volume} and $G_{cohesion}$ being null, which is the case of LEFM. Because of the extreme stress gradients in the LFEM problem, this case probably provides the most severe test of the ability of a FEM mesh to accurately predict G_{tip}. We have found that, using regular meshes of three-noded and four-noded elements, G_{tip} converges to the correct solution with added mesh refinement, even without the use of singularity elements. Furthermore, the accuracy of G_{tip} is relatively unaffected by poorly shaped elements near the crack tip. Our convergence studies have shown that for meshes with all elements approximately the same size, b, the accuracy of the G_{tip} solution depends upon the ratio of element size, b, to least dimension, LD, associated with the crack tip[19]. For b/LD=1, the solution error in G_{tip} is approximately 50%. For b/LD=20, the solution error drops to approximately 10%.

We have also done convergence studies for problems in which $G_{cohesion}$ is non zero(interface elements model a cohesive crack as part of the FPZ energy dissipation). In the problems that we investigated, convergence was achieved with relatively coarse meshes(10% error with meshes having b/LD=0.5).

7. EXAMPLE PROBLEM

To test the method, we have used as an example the plain concrete three-point bend beam tested by Petersson[20]. The relevant properties of that beam are : depth=0.2m, length =2m, thickness=0.05m, tensile strength=3.33MPa, G_f=137N/m, and Young's modulus=30,000MPa.

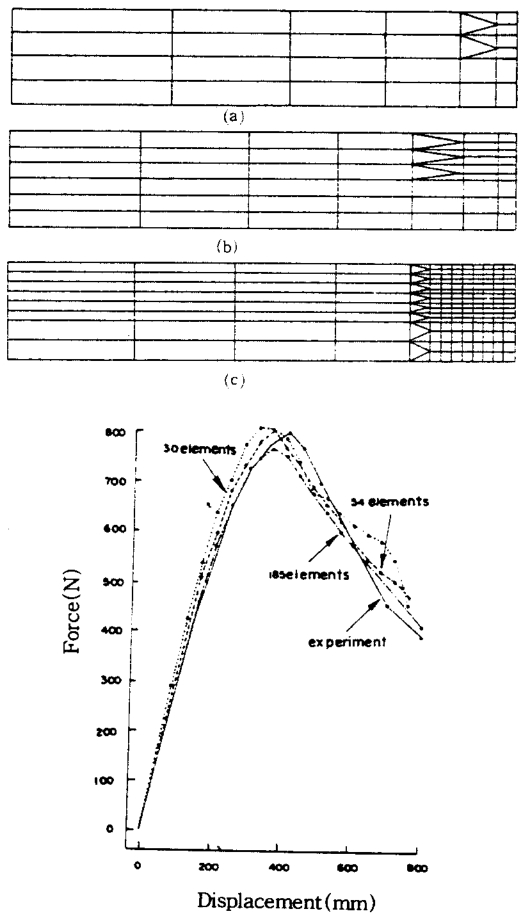

Fig.4 FEM analysis of a three-point beam in bending shows that very coarse meshes are effective in predicting the correct load-displacement curve. Mesh (a) 30 elements, Mesh (b) 54 elements, Mesh (c) 185 elements.

Fig.4 shows three different meshes used to analyze the beam, the load versus load point displacement curves calculated from the three meshes, and the experimental result. In the FEM analyses, we have assumed that $G_{volume}=0$, $G_{cohesion}=G_f$ and $G_{tip(crit)}=0$.

It is clear from Fig.4 that all three meshes produced essentially the same load versus displacement curves, andthat they were all close to the experimental result. The energy absorbed by the beam is given by the area under the load-displacement curve. It is seen that these areas are all approximately the same, and therefore, from a global energy point of view, the method appears to give reasonable results.

In conclusion, a nonlinear, fracture sensitive problem has been solved using a mesh with only 30 linear and bilinear finite elements(73 degrees of freedom), and satisfactory results have been achieved.

8. CONCLUSIONS

The deformation and fracture of salt involves both smeared and discrete cracking mechanisms. To successfully model the behavior of gas-driven hydrofracture at WIPP using FEM, it is necessary to develop a method by which smeared mechanisms and discrete cracking can be modeled simultaneously. We have developed an energy-based approach that combines fracture mechanics and smeared damage mechanics in a consistent manner.

The essence of our approach is to allow modeling to any degree desired of nonlinear, inelastic behavior of the continuum. However, we preclude the development of negative eigenvalues(negative tangent stiffness) in the continuum constitutive relation. Instead, we introduce a discrete crack into the continuum if a zero eigenvalue develops. The discrete crack may be modeled as a cohesive crack or as a cohesionless crack.

The essence of the approach is to calculate that portion of the energy dissipation rate associated with the crack tip, G_{tip}, that is not modeled explicitly by the constitutive relations in the FEM model. Then, to determine if the crack will propagate, we compare G_{tip} to a critical value, $G_{tip(crit)}$, that can be calculated by considering propagation of a steady-state crack in an infinite continuum.

The approach essentially expands the Griffith[1)] energy balance concept to include fracture in inelastic media, the Dugdale-Barenblatt concept, and LEFM in one coherent theory.

We have also presented some aspects the FEM implementation, including the calculation of energy dissipation rates, remeshing to accommodate crack propagation, and convergence considerations.

Finally, we have presented an example problem of Mode I fracture of a concrete beam, including a cohesive crack model.

The goal of FEM modeling of gas-driven hydrofracture in inelastic salt media now appears to be within our grasp. We are in the process of writing a code for this, and other, purposes.

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