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Theory of Explosions in Anisotropic Media

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ABSTRACT

When a suitable process for retorting of oil shale has been devised it will become possible to extract large amounts of kerogen, a potential substitute for oil. We have been studying the mechanics of fragmenting oil shale by means of explosives, with an emphasis on layering effects, and in this report we describe the response of a transversely isotropic material to a spherical explosion. At high pressures the constitutive law is essentially the (isotropic) Mie-Gruneisen equation of state, whereas at lower pressures it approaches an elastic, ideally plastic formulation exhibiting transverse isotropy. Elastic and plastic strain rates are superposed to obtain the total strain rate in the usual fashion. Because we intended to use the constitutive law in a standard continuum computer code, it was necessary to invert the resulting relation to obtain stress rate as a function of strain rate. The resulting constitutive law has been incorporated into the continuum ALE (Arbitrary Lagrangian-Eulerian) computer code, YAQUI. Contrary to our initial expectations, the cavity computed at late times is spherical to within a few per cent. Though at early times the shock wave is also spherical, the effects of anisotropy subsequently become very strong. Tensions that are not present in isotropic media appear near a 45° cone and suggest a new method of fracturing.

I. INTRODUCTION

Vast deposits of oil shale in the western United States could be exploited to solve much of our energy problem if an economical means of processing it were available. One of the most promising approaches is the modified in-situ method, in which a portion of the oil shale is mined out and a large bed of rubble is prepared with explosives. Then combustion supported by forced air causes the organic matter (kerogen) to separate from the rock. A portion of the kerogen supports the flame, and the remainder flows to the bottom of the retort, whence it is pumped out.

Conversion of the competent shale to rubble by means of explosives is complicated by the variability of the shale, which involves natural voids, joints, and faults and is randomly stratified. Still, we think that many systematic features of the process can be investigated by developing a theoretical model and studying its response to explosives by computer simulation. We are particularly interested in the effects of anisotropy and the possibility that anistropy can influence the propagation of shock waves and the subsequent fracture processes. From the theoretical point of view, it is convenient to separate anisotropic effects into three classes. In the elastic regime, the moduli vary with orientation by roughly a factor of 2, and it is relatively straightforward to determine them by acoustic methods. In the plastic regime, the flow stress also varies by a factor of ~2, as determined by triaxial tests. Finally, fractures can propagate under certain combinations of principal stress, and the tensile fracture strength appears to vary with orientation by a factor of 2 to 5.

More important than these effects is the possibility that the entire mechanism of wave propagation and fracture is modified by the anisotropy and that new phenomena appear. We concentrated our first efforts on the effects of spherical charges, because any absence of point symmetry can then be attributed unambiguously to anisotropic effects. Theoretical studies have predicted and experiments confirm that enhanced fracture appears in the neighborhood of a cone that makes an angle of about 45° with the bedding planes. Though in general agreement, many details of this enhanced fracture process differ between theory (in its rudimentary form) and experiments. Of most interest, however, is that enhanced fracture does not exist in isotropic materials and is a clear consequence of the angular dependence of wave propagation.

In this report we show how the associated flow law of plasticity can be used to construct a constitutive law for an ideally elastic-plastic material and how the law can be inverted to provide stress rate as a function of strain rate and stress—an essential step in performing numerical calculations. The resulting constitutive law is used in the YAQUI computer program to compute explosions in a transversely isotropic material, a calculation that requires a two-dimensional (axisymmetric) code. The calculations show that the cavity remains essentially spherical but that tensile hoop stresses develop in the neighborhood of the 45° cone through the center of symmetry. The phenomenon is explained here in terms of wave propagation phenomena.

II. ANISOTROPIC PLASTICITY

If we assume a plastic potential, we can use the associated flow rule to construct a constitutive relation describing plastic flow. In this section we show that the equations can be solved explicitly for the stress rate, even in the case of anisotropic materials. The importance of material rotation is greater for anisotropic than for isotropic materials; consequently, the analysis begins with a discussion of the kinematics of rotation. Next, we construct a potential involving a 4-index plasticity tensor which is a generalization of the scalar yield strength that appears in isotropic plasticity. The flow law involves a Lagrangian multiplier, λ, which we determine as a function of the stress, strain rate, and material properties. Papers discussing plasticity frequently provide expressions for λ that involve the stress rate, but such expressions are not adequate for numerical work because the stress rate is what we need to find. For that reason, the calculation indicated here is somewhat more involved than in the usual treatments. We show that there is no change in plastic volume, in agreement with Hill.[1] Finally, we indicate how the stress can be separated into an isotropic part, which dominates the behavior at high pressures, and an anisotropic part which dominates the low-pressure behavior.

To account for material rotation in the constitutive law, we relate the stress in space axes, σ, to the stress in material axes, $\bar{\sigma}$, through the rotation matrix R by means of the equation

$$\sigma = R\bar{\sigma}R^T \quad , \tag{1}$$

as discussed by Dienes.[2] A similar relation transforms the strain rate matrix, D, into material axes:

$$\bar{D} = R^T D R \quad . \tag{2}$$

Because the constitutive law to be developed expresses stress rate in terms of stress and strain rate, we must consider how the stress rate is affected by rotation. Physically, the state of material stress clearly is not affected by material rotation, but as the material rotates the components of stress in fixed space axes will vary. If we define the rate of material rotation, Ω, by

$$\Omega = \dot{R}R^T \quad , \tag{3}$$

then the result of differentiating (1) can be written

$$\dot{\sigma} = \Omega\bar{\sigma} + \dot{\bar{\sigma}} - \bar{\sigma}\Omega \quad . \tag{4}$$

The quantity

$$\hat{\sigma} = \dot{\sigma} - \Omega\bar{\sigma} + \bar{\sigma}\Omega \tag{5}$$

is the Jaumann-Noll stress rate if Ω represents the vorticity. Reference 2 shows that the quantity Ω given in (3) is approximated by the vorticity for small deformations; hence we may put

$$\Omega = (\omega_{ij}) \quad , \tag{6}$$

where

$$\omega_{ij} = \frac{1}{2}(u_{i,j} - u_{j,i}) \quad . \tag{7}$$

For anisotropic materials we assume the existence of a plastic potential having the form

$$f = \frac{1}{2} b_{ijkl}\sigma_{ij}\sigma_{kl} \quad . \tag{8}$$

By comparison with the expression

$$2f = F(\sigma_y - \sigma_z)^2 + G(\sigma_z - \sigma_x)^2 + H(\sigma_x - \sigma_y)^2$$

$$+ 2L\,\tau_{yz}^2 + 2M\,\tau_{zx}^2 + 2N_{xy}^2 \tag{9}$$

given by Hill, we can deduce the terms of the b_{ijkl} tensor. It is convenient, however, to reduce the number of indices by defining the stresses as a nine-element vector, Σ_K, with the values of K being given by the matrix

$$\begin{array}{c|c} j \backslash i & \begin{array}{ccc} 1 & 2 & 3 \end{array} \\ \begin{array}{c} 1 \\ 2 \\ 3 \end{array} & \begin{pmatrix} 1 & 6 & 4 \\ 7 & 2 & 8 \\ 5 & 9 & 3 \end{pmatrix} \end{array} \quad . \tag{10}$$

Then the plastic potential takes the form

$$f = \frac{1}{2} B_{KL}\Sigma_K\Sigma_L \quad . \tag{11}$$

The elements of the matrix are given by

$$B = \begin{pmatrix} G+H & -H & -G & 0 & 0 & 0 & 0 & 0 & 0 \\ -H & H+F & -F & 0 & 0 & 0 & 0 & 0 & 0 \\ -G & -F & F+G & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & M & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & M & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & N & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & N & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & L & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & L \end{pmatrix} \tag{12}$$

Hill shows that for transversely isotropic materials

$$F = G \quad , \tag{13}$$

$$L = M \quad , \tag{14}$$

and

$$N = F + 2H \quad . \tag{15}$$

This is the case of interest in our numerical calculations, which will assume axially symmetric flow. If we assume that the plastic strain rates can be derived from the plastic potential, f, then

$$D_K^p = \lambda \frac{\partial f}{\partial \Sigma_K} = \lambda B_{KL}\,\Sigma_L \quad . \tag{16}$$

Also, the elastic strain rate for an anisotropic material is given by

$$D_K^e = Q_{KL}\,\hat{\Sigma}_L \quad . \tag{17}$$

The total strain rate

$$D_K = D_K^p + D_K^e \tag{18}$$

is then given by

$$D_K = \lambda B_{KL}\Sigma_L + Q_{KL}\hat{\Sigma}_L \quad . \tag{19}$$

If we define

$$C = Q^{-1} \tag{20}$$

and express the relation for D_K in matrix notation as

$$D = \lambda B\Sigma + Q\hat{\Sigma} \quad , \tag{21}$$

then we can solve for $\hat{\Sigma}$

$$\hat{\Sigma} = C(D - \lambda B\Sigma) \quad . \tag{22}$$

We can write the stress rate as

$$\hat{\Sigma}_K = \dot{\Sigma}_K + T_K \quad , \tag{23}$$

where

$$t_{ij} = \sigma_{im}\omega_{mj} + \sigma_{mj}\omega_{mi} \tag{24}$$

and the T_K vector is related to the t_{ij} matrix in the same manner as previously indicated for the stresses and strain rates. Then (22) reduces, in matrix rotation, to

$$\dot{\Sigma} = C(D - \lambda B\Sigma) - T \quad . \tag{25}$$

To determine λ we note that when the yield condition

$$\frac{1}{2} B_{KL}\Sigma_K\Sigma_L = 1 \tag{26}$$

is differentiated we obtain the relation

$$B_{KL}\Sigma_K\dot{\Sigma}_L = 0 \tag{27}$$

involving $\dot{\Sigma}_L$. In combination with (25) we can obtain an expression for the Lagrangian multiplier

$$\lambda = \frac{G_{LM}\Sigma_L D_M - \gamma}{H_{LN}\Sigma_L\Sigma_N} \quad , \tag{28}$$

where

$$H_{LN} = B_{KL}B_{MN}C_{KM} \quad , \tag{29}$$

$$G_{LM} = B_{KL}C_{KM} \quad , \tag{30}$$

and

$$\gamma = B_{KL}\Sigma_L T_K \quad . \tag{31}$$

The rotational contribution, γ, can be expressed as the sum of two terms

$$\gamma_1 = b_{ijkm}\sigma_{il}\sigma_{km}\omega_{lj} \tag{32}$$

and

$$\gamma_2 = b_{ijkm}\sigma_{lj}\sigma_{km}\omega_{li} \quad . \tag{33}$$

In the case of current interest the rotation is about a fixed axis as the result of axial symmetry of the problem, and only the terms ω_{13} and ω_{31} do not vanish. Then, if we write

$$\omega_{13} = \Omega \tag{34}$$

we find

$$\gamma_1 = \gamma_2 = [(H + 2F - L)\Sigma_1 - (H - F)\Sigma_2 + (L - 3F)\Sigma_3]\Sigma_4\Omega \quad , \tag{35}$$

hence

$$\gamma = 2\gamma_1 \quad . \tag{36}$$

For isotropic materials,

$$L = M = N = 3F = 3G = 3H \tag{37}$$

as discussed by Hill. Consequently,

$$\gamma = 0 \quad . \tag{38}$$

To show that the rate of change of plastic volume is zero we write

$$\dot{\theta}^P = d^P_{ii} = \lambda b_{iikl}T_{kl} \quad . \tag{39}$$

In the reduced index notation (39) can be expressed as

$$\dot{\theta}^P = \lambda(B_{1J} + B_{2J} + B_{3J})\Sigma_J \quad . \tag{40}$$

However, for any J, the sum of the first three terms in a row of the B matrix given as (12) is zero; consequently,

$$\dot{\theta}^P = 0 \quad , \tag{41}$$

demonstrating that the theory does not allow for permanent changes in volume.

At high pressure the stress is essentially that associated with the Mie-Gruneisen equation of state

$$p = p(\rho, I) \quad , \tag{42}$$

where ρ is the material density and I the specific internal energy. At intermediate pressures the stress can be expressed as

$$\sigma_{ij} = \sigma^L_{ij} - (p - k\mu)\delta_{ij} \quad , \tag{43}$$

where σ^L_{ij} denotes the low-pressure component of stress determined in the preceding pages and $p - k\mu$ is the excess of the pressure over the linear approximation. Otherwise expressed,

$$\text{stress} = \begin{pmatrix}\text{low-pressure}\\ \text{component of}\\ \text{stress}\end{pmatrix} + \begin{pmatrix}\text{high-pressure}\\ \text{component of}\\ \text{stress}\end{pmatrix} - \begin{pmatrix}\text{common}\\ \text{part}\\ -k\mu\,\delta_{ij}\end{pmatrix} .$$

Here the compression is expressed as

$$\mu = 1 - \rho_o/\rho \quad . \tag{44}$$

III. ANISOTROPY FRAGMENTATION

Lagrangian codes determine the movements in a continuum by tracking elements of mass with the momentum equation

$$\rho\dot{u}_i = \sigma_{ij,j} \tag{45}$$

Though YAQUI[8] is an Arbitrary Lagrangian-Eulerian Code, for oil-shale calculations it can be made to function as a Lagrangian code by a special choice of the mesh-moving equations. We resist discussing the finite-difference method here, focusing on the physical interpretation of the numerical results.

The effects of a spherical charge of explosive can be approximated by representing the charge as a sphere of uniform, polytropic gas with index 3. Although the transit time of the detonation wave initiated at the center is neglected, the average value of the pressure at the interface is approximated well by this simplification. The cavity remains spherical to within a few per cent when the best estimates of oil-shale elastic and plastic properties are made. The elastic parameters for 2 g/cm[3] material are,[4] in GPa,

$$C_{11} = 24.5,\ C_{33} = 15.1,\ C_{44} = 5.1,\ C_{66} = 8.0,\ C_{12} = 8.5,\ C_{13} = 6.2\ . \tag{46}$$

The variation of strength with bedding angle is given in Fig. 1, which shows that the plasticity theory used to model the triaxial test results of McLamore and Gray[5] gives a minimum strength at 45°, whereas the test results indicate the minimum at 60°. It is not clear whether the discrepancy represents a defect of the theory or of the test method, which tends to cause failures across the diagonal of the specimen. Because the test specimens have an aspect ratio of 2 when the bedding angle is 60° (Fig. 1), the diagonal coincides with the bedding plane, and the coincidence may contribute to the experimental

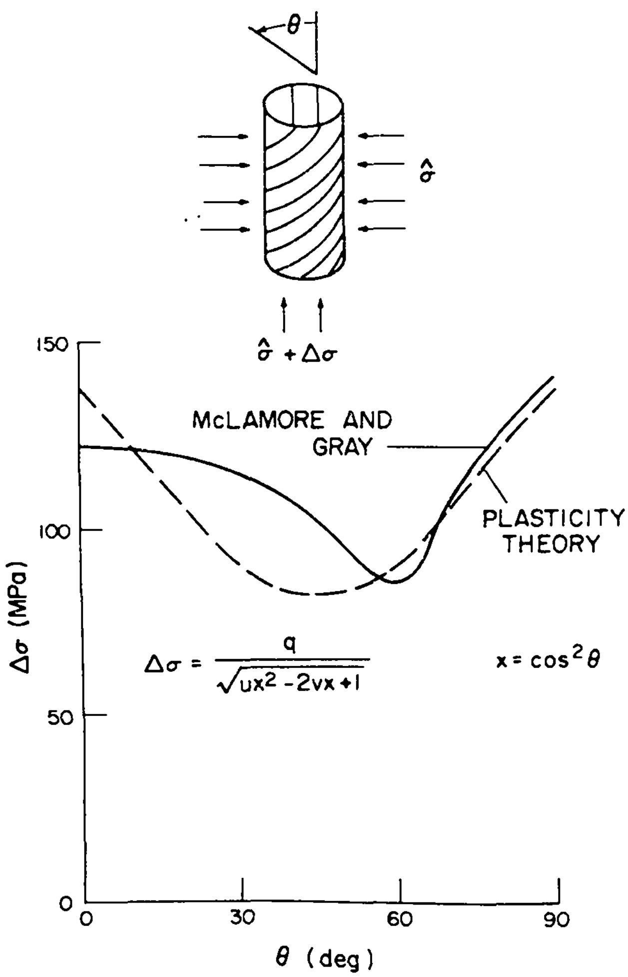

Fig. 1.
Comparison of theoretical and measured strength-vs-orientation curves (the latter from data of McLamore and Gray, Ref. 5).

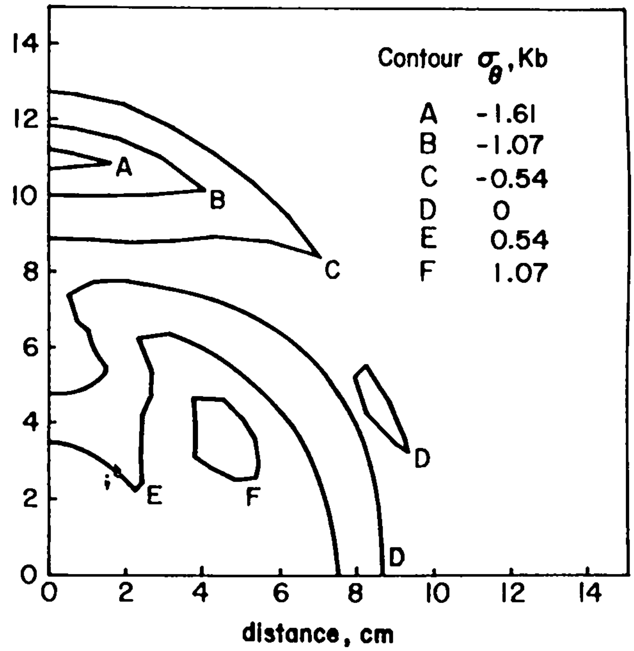

Fig. 2.
Contours of constant hoop stress $\sigma_{\theta\theta}$ at 43 μs resulting from a spherical detonation in anisotropic oil shale.

minimum at 60°. The high-pressure constitutive law takes its form from the empirical relation[6]

$$u_S = C + Su_p \tag{47}$$

between shock velocity and particle velocity. This, together with the constitutive law defined above, defines the theoretical behavior of the shale.

The effect of bedding on material strength, illustrated in Fig. 1, can be understood by considering a stack of plates of elastic-plastic material separated by a lubricating material of lower strength. When stressed in compression by loads in either the vertical or horizontal direction, the stack has the same strength as the plate material, but when a core with an axis at 45° to the vertical is loaded along its axis, the strength is reduced because of slip along the bedding planes.

The result of a spherical explosion is illustrated in Fig. 2, which shows contours of the hoop stress $\sigma_{\theta\theta}$. This principal stress is associated with the directions normal to planes through the axis of symmetry of the problem. Tensile values of $\sigma_{\theta\theta}$ tend to cause failures analogous to the separation of orange sections. In an explosion in an isotropic medium the stress contours are spheres and the stresses are all compressive out to very large radii. The effect of anisotropy is to cause a region of tensile hoop stress centered at about 5 charge radii from the center of the explosive. The tensile stresses exceed a kilobar over a significant region, and half a kilobar over a large volume.

In a spherical explosion in horizontally bedded material the upper portion of the wave front (which is approximately spherical) is attenuated at a rate that depends on the vertical strength, and the horizontal wave front attenuates at essentially the same rate because it enters material that appears to have the same strength. Analytic solutions for spherical waves have been discussed by Luntz,[7] Chadwick and Morland,[8] and Blake and Dienes,[9] but in realistic calculations material nonlinearities in the oil shale and the complexities of the pressure history in the explosive make analytic solutions intractable. Intuitively, one expects the wave to attenuate more rapidly where the strength is higher, and that is borne out by the calculations in spherical geometry illustrated in Fig. 3, where the stress profiles for spherical waves in isotropic shales having shear strengths of 0.05 and 0.0913 GPa are compared. Because the wave moving along a 45° cone in an anisotropic shale encounters material of apparently lower strength than the horizontal and vertical waves, it attenuates more slowly. Consequently, the hoop stress in the vertical plane is greatest on the 45° cone, and it causes material to move away from the cone. Though the effect is relatively small in terms of stress gradients, it is large enough to cause a small reduction in residual density, leaving a residual tensile stress that exceeds a kilobar in certain regions. We estimate that the volume of the toroidal tensile region is about 60 times the volume of the charge.

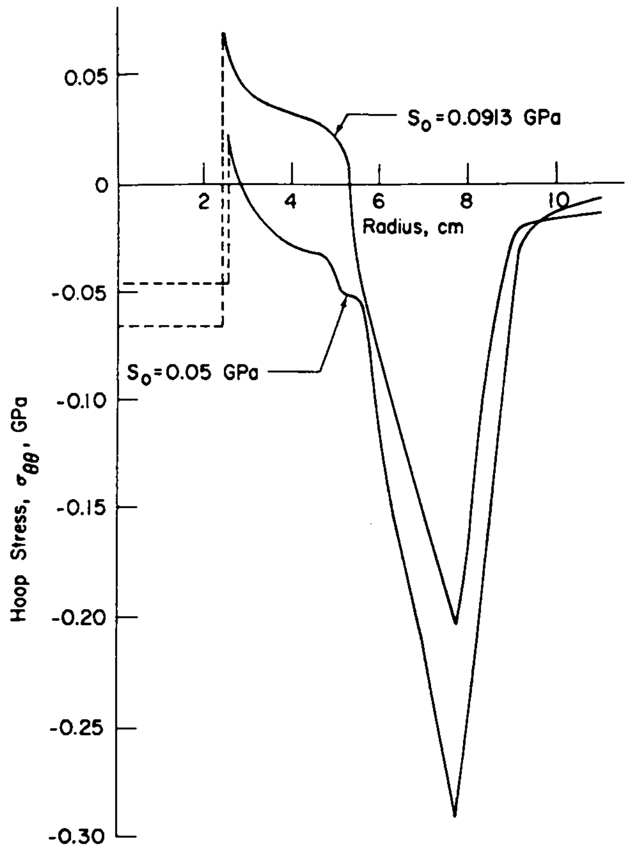

Fig. 3.
Profiles of spherical waves in isotropic shales with shear strengths (S_o) of 0.05 and 0.0913 GPa.

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