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COMPUTER PROGRAM UKO

A. Edward Ratcliffe
John W. White

March 29, 1973

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Preface

UKO is a computer program (or code) that uses the finite difference method to solve initial-value problems of continuum rock mechanics in one spatial dimension. Planar, cylindrical, and spherical symmetries are allowed. All media are assumed to be isotropic and homogeneous. The name UKO, an acronym for "Underground KO," was chosen to indicate that the code was developed from the KO code¹ and deals with rock mechanics. KO simulates elastic behavior and plastic flow.

Rock behavior is considerably complicated by the failure processes that occur as stress waves traverse rock media. UKO extends the KO computer program to include models to simulate the brittle/ductile failure associated with rocks. Models also describe the very general failure surfaces of rock, how these surfaces change, and how stresses relax or are limited during failure. Also used in UKO is a new form of artificial viscosity that provides smoother and more accurate solutions.

The purpose of this report is to provide the user of UKO with a general description of the models used and to show how these models are represented in the coding. We hope that the user who reads this report and the UKO Input Description carefully will find the code to be, not a black box, but a light gray box that he can use with ease and confidence.

The user should be warned that UKO simulates processes that are complex and subtly interrelated. Nevertheless, UKO gives the user exceptional freedom in specifying equation of state information so that a very wide range of materials and states can be represented. When improperly used, this freedom can lead to nonsensical results. For these reasons it is imperative that the user understand the models of the code before he uses it for quantitative predictions. No code can outguess its users, nor can it always fail safely.

COMPUTER PROGRAM UKO

Part I: Modeling

INTRODUCTION

The basic equations of continuum mechanics are the conservation equations of mass, momentum, and energy; in addition, one must have an equation-of-state (EOS) of the materials. For purely hydrodynamic (fluid) systems, the EOS can be just the expression of pressure as a function of energy (or temperature) and density. Such use of pressure alone is limited to materials for which the stress field is always isotropic, i.e., the force per unit area at a point is the same in every direction. Solid materials cannot be characterized in this manner, because, in addition to resisting changes in density, they have the additional property of resisting changes in shape.

In this document we assume that the reader is familiar with purely hydrodynamic behavior and the use of pressure as a variable used to characterize such behavior. We also assume that the reader is familiar with the notion of approximating differential equations by finite difference equations. In Part I, we present an elementary discussion of elastic behavior and numerical considerations, but we emphasize the failure description of the UKO code. We encourage the reader to read Wilkins' paper (Ref. 1).

ELASTIC BEHAVIOR

For any given infinitesimal element in an isotropic medium, it is possible to characterize the stress state by six components: σ_x , σ_y , σ_z , τ_x , τ_y , and τ_z . Only three of these are independent (Fig. 1).

The components σ_i ($i = x, y, z$) represent the stress normal to the face of the element whose face is perpendicular to the i -axis; the shear stresses (τ_i , not shown in Fig. 1) are stresses parallel to the same element face. It is always possible, by rotation, to find a coordinate system for which all the τ 's are zero; this is called the principal coordinate system. It is convenient, though not necessary, to discuss the stresses with respect to the principal coordinate system, so the stress description in the rest of this document assumes the

Fig. 1. Stresses normal to an infinitesimal volume.

principal coordinate system. Let σ be positive for a stress directed out from the differential element. We separate the stress σ_i into an isotropic component P (pressure) and a deviatoric component S_i .

$$P = -1/3 (\sigma_1 + \sigma_2 + \sigma_3)$$

$$S_i = P + \sigma_i.$$

Thus the pressure is just the negative of the average stress, and the i th deviatoric stress is just the difference between the i th principal stress and the average stress. In UKO, changes in density are associated with pressure, and changes in shape are associated with the deviatoric stresses.

In Fig. 2, a shear stress τ is applied to an elastic solid. In elastic behavior, the solid returns to its original rectangular shape after τ is removed. We define the shear strain in this system as δ , the tangent of the angle ψ . The material parameter of most interest in determining δ is the modulus of rigidity G (also called the shear modulus), which is defined as

Fig. 2. Shear distortion of an infinitesimal volume. ψ is an infinitesimal angle.

$$G = \frac{\tau}{\delta} = \frac{\text{shear stress}}{\text{shear strain}}.$$

G is a measure of the degree to which a material can support anisotropic stresses. Thus, for hydrodynamic fluids, for which the stresses are always isotropic, $G = 0$. Likewise, G is also a measure of the degree to which a material resists changes in shape. In the UKO computer code, the user specifies G as a function of pressure.

The material description must also include the manner in which the material resists change in density. This is required for both hydrodynamic fluids and solids. Then

$$\frac{dV}{V} = -\frac{dP}{K},$$

where K is the bulk modulus. A large value of K indicates that the material is hard to compress. We note also that

$$\frac{dV}{V} = \epsilon_1 + \epsilon_2 + \epsilon_3,$$

where ϵ_i is the strain of elongation of the i th direction, $(\Delta l/l)_i$.

In the UKO code, it proves most convenient to obtain the pressure directly from an EGS in which the pressure is a function of density and energy. However, the deviatoric stresses are obtained by integrating the following equation (from Wilkins¹):

$$\dot{S}_i = 2 G (\dot{\epsilon}_i - 1/3 \dot{V}/V),$$

where the dot denotes time derivative. To this point, the behavior has been assumed to be elastic. To complete the description for rocks, failure must be included.

BRITTLE/DUCTILE FAILURE

When material fails, the stresses are relaxed (reduced in size) or their growth is limited. Before discussing this aspect of failure, we require a criterion to determine when such failure mechanisms are to occur. To discuss this criterion, we express the stress state in terms of invariants. There can be three independent invariants for any given description of a stress state. These invariants may be, of course, expressed in terms of $\sigma_x, \sigma_y, \sigma_z, \tau_x, \tau_y$, and τ_z . Again, our discussion is confined to the principal coordinate system for which the τ 's are zero. One such possible set (a standard one) of invariants follows:

$$\begin{aligned} I_1 &= \sigma_1 + \sigma_2 + \sigma_3 && \text{First invariant} \\ I_{2D} &= 1/2 (\sigma_1^2 + \sigma_2^2 + \sigma_3^2) && \text{Second deviatoric invariant} \\ I_{3D} &= \sigma_1 \sigma_2 \sigma_3 && \text{Third deviatoric invariant} \end{aligned}$$

For a more detailed discussion of invariants, the reader is referred to the books by Nadai,² Jaeger,³ Liebowitz,⁴ and Jaeger and Cook.⁵ For convenience, in the UKO code we use the following invariants:

$$\begin{aligned} P &= -1/3 I_1 && (\text{pressure}) \\ \tau_o &= \sqrt{2/3 I_{2D}} && (\text{octahedral shear stress}) \\ I_{3D}^{1/3} & && \end{aligned}$$

Note that they all have units of stress. The octahedral shear stress is the shear stress on the face of a differential element when that face is rotated so it is equally inclined to the principal axes. The expression $I_{3D}^{1/3}$ is a measure of the relative values of the stresses. For example, $I_{3D}^{1/3} = 0$ when the greatest principal stress exceeds the average stress by the same amount that the least stress is less than the average stress. This is equivalent to saying that, for $I_{3D}^{1/3} = 0$, the stress state is a pure shear superimposed on a pressure. We define compression as those stress states for which

$$\sigma_1 < \sigma_2 = \sigma_3 .$$

We define extension as those stress states for which

$$\sigma_1 = \sigma_2 < \sigma_3 .$$

It can be shown that, for compression and extension,

$$\tau_o = \pm \frac{2^{1/2}}{2^{1/3}} I_{3D}^{1/3}$$

By examining a cross section of the $P, \tau_o, I_{3D}^{1/3}$ space for constant P , we can see how the compression extension cases bound the stress space. Also, we note how a failure curve separates failed stress states from unfailed stress states (Fig. 3). (For further details regarding this stress space, see Ref. 6). Note that the failure curve in the above figure becomes a failure surface when extended in the direction of the pressure axis. Experiments on rocks are frequently reported in a curve of τ_o versus P for several test types (i.e., compression, extension, and $I_{3D}^{1/3} = 0$), as shown in Fig. 4. The $I_{3D}^{1/3} = 0$ case is usually denoted by the name "torsion," since it is obtained by twisting thin-walled cylinders under hydrostatic pressure.

In Fig. 4, these curves have been extended by dashed lines to estimate what the complete failure surface might look like in those regions where data are usually unavailable. At high pressures, the material behaves in a ductile manner and all test types would have the same value of τ_o at failure. At extremely high pressure, τ_o must come to zero as the material melts and can no longer

sustain shear stresses. For negative pressures (tension), typical materials are quite weak. We assume that all the curves converge to the same point ($\tau_o = 0$) on the pressure axis for which the material is in hydrostatic tension. To generate the complete failure surface from the graph of Fig. 4, we can assume that τ_o is expressible as a three-termed expansion in terms of $I_{3D}^{1/3}$ for any given value of P . Then the coefficients in the expansion are functions of pressure only. The failure surface is then given by

$$\tau_o (\text{failure}) = A_1(P) + A_2(P) I_{3D}^{1/3} + A_3(P) I_{3D}^{1/3} \quad (1)$$

This technique generates a fairly general class of failure surfaces. We use this approach in UKO, although the third (A_3) term is eliminated because two of the

Fig. 3. $\tau_o - I_{3D}^{1/3}$ cross section of the stress space. All possible stress states are within the semi-infinite trough. Possible unfailed states lie below the failure curve.

Fig. 4. $\tau_o - P$ projection of the stress space.

principle stresses are always equal in a one-dimensional computer code (the stress state is always compression or extension). The failure surface is specified in the UKO code by specifying values of τ_o as a function of pressure both for compression and extension. The code then generates the pressure-dependent coefficients, A_1 and A_2 , of Eq. (1).

So far, we have discussed only the mathematical mapping of a failure surface. It should be emphasized that the model assumes that failure is a function of the stress state only, and is independent of path. We must now provide a computational model that simulates stress behavior during failure.

We begin by assuming that there exists a continuum of failure surfaces that depend on the state of material. The continuum is bounded by two extremes: a failure surface for consolidated material and a failure surface for rubble. UKO requires that these two bounding failure surfaces be given. All material is assumed to be initially consolidated. At failure, however, the surface changes to some value intermediate between consolidated and rubble. To determine this intermediate surface for each material, RUBF (rubble fraction) is specified in UKO as a function of the pressure at which failure occurs. Thus, for most materials, RUBF = 1 for failure at negative pressures, and RUBF might be expected to approach 0 as the pressures get large and the rock behaves in a fairly ductile manner. If we assume that τ_o (at failure) is independent of $P^{1/3}_D$ and that the three types give the same $\tau_o - P$ relationship, then Fig. 5 shows what these surfaces might look like in a $\tau_o - P$ plot. Note that the rubble surface has been indicated as possessing no strength for negative pressure. If an element of material in Fig. 5 goes from A to B in one time step, the new failure surface is far from B and the stresses must be relaxed. On the other hand, if $P > P_D$, the material may be ductile and one might simply limit τ_o so that it cannot go above the failure surface.

Fig. 5. Comparison of consolidated and rubble failure surfaces.

Brittle behavior will be defined as the low-pressure stress-relaxation process. Wilkins⁷ has suggested that computer codes can use two simple models (dislocation and Maxwell solid) for stress relaxation. UKO also uses a dislocation model in which τ_o is reduced at a constant rate

$$\dot{\tau}_o = -2G\dot{\gamma} ,$$

where $\dot{\gamma}$ (the plastic strain rate) is input to UKO for each material. UKO also uses a modified Maxwell solid model for stress relaxation for brittle failure,

$$\dot{\tau}_o = -\frac{G}{\eta} \Delta \tau_o ,$$

where $\frac{1}{\eta}$ (inverse viscosity) is input for each material, and where $\Delta\tau_0$ is the difference between the value of τ_0 and the failure surface value of τ_0 at the same value of P . This simply says that the relaxation rate becomes faster as the stress state is farther from the failure surface.

The values of $\dot{\gamma}$ and η^{-1} determine brittle failure stress relaxation rates. However, for ductile failure we simply limit τ_0 so it cannot go above the failure surface. DUCF (ductile fraction) is input to UKO as a function of pressure to determine the mixture of failure mechanisms. One might have DUCF = 0 for low pressure, and the value of DUCF would go smoothly to 1 as the pressure increases.

In UKO, material melts when a specified specific energy occurs for a given material. As this energy value is approached, the purely solid-like properties of the material vanish. Thus the shear modulus (G), the deviatoric invariants (τ_0 and I_3^D), and the failure surface all approach zero.

When material spalls, the pressures and stresses both relax completely and the shear modulus is set to zero. The UKO code assumes that spall occurs when the specific volume of material exceeds the value of specific volume associated with the minimum pressure that can be sustained by the material according to the failure surface. As material recompacts and positive pressures are achieved, the degree of ductile behavior is used as a criterion to allow the shear modulus to heal so that its full value is regained when the ductility reaches a specified value. The P-V data is then used to calculate the corresponding volume for spall. This spall volume is also used as a criterion for recompaction. If the material recompacts, then it becomes necessary to use the P-V data again. It should be noted that the spalling phenomenon involves discontinuous behavior when spalled material is recompacted. We have found that the undesirable noise in the solution for recompaction of spalled material is reduced by the use of artificial viscosity (see "Numerical Considerations"). Typically, a linear q multiplier equal to 0.5 is used for spalled material.

A number of idealized test problems have been run in which the methods of mixing the failure surfaces (consolidated/rubble) and failure mechanisms (brittle/ductile) have been varied over reasonable ranges. The resulting variations of velocity fields, displacements, etc., in such calculations have been very small.

The code provides smooth and continuous material behavior (with the exceptions of spall), and solutions converge as zone size is reduced. The scale of the failure description is macroscopic rather than microscopic, and a continuum-mechanics model is used. However, the flexible input format allows the code user to input EOS information in a physically inconsistent way and to include discontinuities in these EOS's. Thus, as is true with almost all computer programs, the code user must appreciate the limits of the model before he can use it profitably. To simulate a real shock wave and the subsequent relaxation, one would need to model the real viscosity (rather than artificial viscosity) and have the zone size small compared to the shock-rise thickness. Then one could also use physically measured values for relaxation rate constants. Unless this is done, the relaxation mechanisms must be considered

as numerical artifices and close "cousins" of the artificial viscosity. Thus, it may be necessary to determine $\dot{\gamma}$ and η^{-1} by trial and error to obtain a smooth (non-noisy) solution. In a wide variety of test problems, however, it was observed that the calculations were not significantly affected by varying $\dot{\gamma}$ and η^{-1} over several orders of magnitude. This indicates that the dominant numerical artifice is the artificial viscosity, which is discussed in "Numerical Considerations."

Because of the artificial nature of $\dot{\gamma}$ and η^{-1} , we have found it useful to bypass the brittle description described above for some calculations. This is done by setting $DUCF = 1$ for all pressure values. Brittle behavior is then designated as the behavior associated with failure that is accompanied by the generation of a new failure surface. Both models are available to the code user, who must determine which is more appropriate for his calculation.

We made UKO calculations (see Appendix) of the Lawrence Livermore Laboratory cratering experiment Pre-Schooner II. Since the code UKO is one-dimensional, the calculation is valid only up to the time at which surface spall occurs. The measured spall (jump-off) velocity was 3.9 cm/m sec, and the calculated velocity was 4.0 cm/m sec. This agreement is satisfactory when one considers the inhomogeneous nature of earth materials and the limited information available regarding their EOS's.

NUMERICAL CONSIDERATIONS

This section deals mostly with the numerical technique called artificial viscosity. This method was proposed by Von Neumann and Richtmyer⁸ to enable the finite difference equations to simulate the physics associated with shocks. The artificial-viscosity method converts the discontinuous functions associated with shocks into rapidly changing (but continuous) functions that the finite-difference method can handle readily. The following form of the so-called "quadratic q" was proposed by Von Neumann and Richtmyer:

$$q = \rho(C_1 \Delta X)^2 \left| \frac{\Delta u}{\Delta X} \right|^2 \quad \left\{ \begin{array}{l} \text{For zones being compressed;} \\ \text{otherwise, } q = 0 \end{array} \right.$$

where ρ is density, C_1 is a constant, ΔX is zone size, and u is velocity. The q is added to the pressure for each equation in which the pressure appears. (Note that the q depends on the zone size in such a way that it vanishes as the zone size approaches zero.) The effect of the q is to provide viscous damping over a few zones where $\Delta u / \Delta X$ is very large. One of the attractive (and necessary) features of this q is that the Rankine-Hugoniot conditions are preserved for shock descriptions, provided that the preshock and postshock values are not in the few zone regions over which the shock has been artificially spread. The UKO code uses an improved form of q described in Refs. 9 and 10. For the quadratic form we have the following q

$$q = \rho(C_1 \Delta X)^2 \left| \frac{\Delta u}{\Delta X} \right| \sqrt{\left| \frac{\Delta p}{\Delta X} \right| \left| \frac{1}{C_s} \frac{\Delta p}{\Delta t} \right|} \quad \left\{ \begin{array}{l} \text{For zones being compressed;} \\ \text{otherwise, } q = 0 \end{array} \right.$$

where p is pressure and C_s is sound speed. This form is more uniquely associated with shocks and provides smoother, more accurate calculations.

The effect of viscosity (real or artificial) is to convert kinetic energy into internal energy. Thus, it affects the solutions of physical problems. The quadratic q is such that it introduces insignificant errors for almost all physical systems. Thus, it is not necessary to let ΔX approach zero to obtain a reasonably accurate computation. For elastic solids, unfortunately, the quadratic q does not provide sufficient smoothing for shocks. Therefore, we add a linear q of the general form

$$q = \rho(C_2 \Delta X) C_s \left| \Delta u \right|.$$

This form is considerably less sensitive to the steepness of gradients. The result is that, in order to smooth the shock region, much more dissipation (nonphysical) is introduced into the calculation as a whole. It is frequently necessary to examine the solution as a function of zone size so that the physical answer can be obtained by extrapolating to the case for $\Delta X = 0$. Since most rock mechanics calculations currently require a linear q , it is essential that the UKO code user be aware of the effect of this artifice. The code user is urged to be familiar with Refs. 8, 9, and 10. For introductory information regarding other methods of handling shocks, the reader is referred to the text by Richtmyer and Morton.¹¹

Part II: Numerical Scheme

INTRODUCTION

In the following sections we present, first, the difference equations of UKO. Most of these are taken directly from KO, are derived and discussed in Refs. 1 and 7, and need no further attention here.

Next, we give the logical structure of the entire code, with a few remarks on the location and order of the difference equations and EOS's in the code.

This is followed by a Fortran listing of the important equations that were changed or added in the transformation from KO to UKO: i.e., the equations of artificial viscosity and of the failure model. These constitute the basic differences between the two codes. The listing is included so that a user may familiarize himself with these new features in complete detail.

We provide a glossary for the names in the Fortran listing.

Copies of the code may be made available to interested organizations outside ILL. However, a review and release procedure is required before the code can be transmitted outside the Laboratory.

OUTLINE OF FINITE DIFFERENCE EQUATIONS OF UKO

Mass Zoning

The material is divided into mass intervals:

$$m_{j+(1/2)} = \frac{\rho_0}{V_0} \left[\frac{(r_{j+1}^0)^d - (r_j^0)^d}{d} \right] \quad \begin{array}{ll} \text{plane:} & d = 1 \\ \text{cylindrical:} & d = 2 \\ \text{spherical:} & d = 3 \end{array}$$

$$j = 1, 2, \dots, N$$

Equation of Motion

$$U_j^{n+(1/2)} = U_j^{n-(1/2)} + \frac{\Delta t^n}{\phi_j^n} \left[(\Sigma_r)_j^{n+(1/2)} - (\Sigma_r)_j^{n-(1/2)} \right] + \Delta t^n (\beta_j^n)(d-1),$$

where

$$(\Sigma_r)_j^{n+(1/2)} = \left\{ -[P^n + q^{n-(1/2)}] + s_1^n \right\}_{j+(1/2)}$$

$$(\Sigma_\theta)_j^{n+(1/2)} = \left\{ -[P^n + q^{n-(1/2)}] + s_2^n \right\}_{j+(1/2)}$$

$$\phi_j^n = \frac{1}{2} \left\{ \rho_{j+(1/2)}^0 \left[\frac{r_{j+1}^n - r_j^n}{v_{j+(1/2)}^n} \right] + \rho_{j-(1/2)}^0 \left[\frac{r_j^n - r_{j-1}^n}{v_{j-(1/2)}^n} \right] \right\}$$

$$\beta_j^n = \frac{1}{2} \left\{ \left[\frac{(\Sigma_r)_{j+(1/2)}^n - (\Sigma_\theta)_{j+(1/2)}^n}{\frac{1}{2}(r_{j+1}^n + r_j^n)} \right] \left(\frac{v^n}{\rho_0} \right)_{j+(1/2)} + \left[\frac{(\Sigma_r)_{j-(1/2)}^n - (\Sigma_\theta)_{j-(1/2)}^n}{\frac{1}{2}(r_j^n + r_{j-1}^n)} \right] \left(\frac{v^n}{\rho_0} \right)_{j-(1/2)} \right\}.$$

At an outside regional boundary J,

$$\phi_J^n = \frac{1}{2} \rho_{J-(1/2)}^0 \left[\frac{r_J^n - r_{J-1}^n}{v_{J-(1/2)}^n} \right]$$

$$\beta_J^n = \left[\frac{(\Sigma_r)_{J-(1/2)}^n - (\Sigma_\theta)_{J-(1/2)}^n}{\frac{1}{2}(r_J^n + r_{J-1}^n)} \right] \left(\frac{v^n}{\rho_0} \right)_{J-(1/2)}.$$

At an inside regional boundary J,

$$\phi_J^n = \frac{1}{2} \rho_{J+(1/2)}^0 \left[\frac{r_{J+1}^n - r_J^n}{v_{J+(1/2)}^n} \right]$$

$$\beta_J^n = \left[\frac{(\Sigma r)_{J+(1/2)}^n - (\Sigma \theta)_{J+(1/2)}^n}{\frac{1}{2} (r_J^n + r_{J+1}^n)} \right] \left(\frac{v^n}{\rho^0} \right)_{J+(1/2)} .$$

For a free surface at $j = J$, the stresses are set to zero at $J + (1/2)$ for an outside free surface or at $J - (1/2)$ for an inside free surface.

$$r_j^{n+1} = r_j^n + U_j^{n+(1/2)} \Delta t^{n+(1/2)} .$$

Equation of Continuity

$$v_{j+(1/2)}^{n+1} = v_{j+(1/2)}^n + \Delta t^{n+(1/2)} \left(\frac{\rho^0}{m} \right)_{j+(1/2)} \left\{ U_{j+1}^{n+(1/2)} \left[r_{j+1}^{n+(1/2)} \right]^{d-1} - U_j^{n+(1/2)} \left[r_j^{n+(1/2)} \right]^{d-1} + \left[x_{j+(1/2)}^{n+(1/2)} \right]^* \right\}$$

$$\eta_{j+(1/2)}^{n+1} = \frac{1}{v_{j+(1/2)}^{n+1}} ; \text{ here, } r_{j+1}^{n+(1/2)} = \frac{1}{2} (r_{j+1}^{n+1} + r_{j+1}^n) , \text{ etc.}$$

$$\left[x_{j+(1/2)}^{n+(1/2)} \right]^* = \frac{[\Delta t^{n+(1/2)}]^2}{12} \left\{ \left[U_{j+1}^{n+(1/2)} \right]^3 - \left[U_j^{n+(1/2)} \right]^3 \right\} .$$

Velocity strains:

$$(\epsilon_1)_{j+(1/2)}^{n+(1/2)} = \frac{U_{j+1}^{n+(1/2)} - U_j^{n+(1/2)}}{r_{j+1}^{n+(1/2)} - r_j^{n+(1/2)}}$$

$$\epsilon_2 = 0 \text{ for } d = 1 .$$

$$(\epsilon_2)_{j+(1/2)}^{n+(1/2)} = \frac{U_{j+1}^{n+(1/2)} + U_j^{n+(1/2)}}{r_{j+1}^{n+(1/2)} + r_j^{n+(1/2)}}$$

* Correction term for $d = 3$ only.

Artificial Viscosity

Linear q:

$$q_{j+(1/2)}^{n+(1/2)} = C_L C_s^{n+1} \rho_{j+(1/2)}^{n+(1/2)} \sqrt{[U_j^{n+(1/2)} - U_{j+1}^{n+(1/2)}]} \\ \sqrt{\left| \frac{(\Delta P)_{j+(1/2)}^n (\Delta X)_{j+(1/2)}^{n+1} \left(\frac{\Delta 1}{\rho} \right)_{j+(1/2)}^{n+(1/2)}}{C_s^{n+1} [\Delta t^{n+(1/2)}]} \right|}^{1/2}$$

Quadratic q:

$$q_{j+(1/2)}^{n+(1/2)} = C_0^2 \rho_{j+(1/2)}^{n+(1/2)} [U_j^{n+(1/2)} - U_{j+1}^{n+(1/2)}] \\ \sqrt{\left| \frac{(\Delta P)_{j+(1/2)}^n (\Delta X)_{j+(1/2)}^{n+1} \left(\frac{\Delta 1}{\rho} \right)_{j+(1/2)}^{n+(1/2)}}{C_s^{n+1} [\Delta t^{n+(1/2)}]} \right|} .$$

where

C_L and C_0^2 are dimensionless constants
 C_s is sound speed
 ΔX is zone size
 ΔP is spatial pressure change
 Δu is velocity gradient
 ρ is density.

Hydrostatic Pressure and Energy

$$P_{j+(1/2)}^{n+1} = A [\eta_{j+(1/2)}^{n+1}] + B [\eta_{j+(1/2)}^{n+1}] E_{n+(1/2)}^{n+1} .$$

The change in internal energy, ΔE , is composed of a hydrodynamic component and a distortion component:

$$\Delta E = -(P + q) \Delta V + \Delta Z .$$

Change in distortion energy, ΔZ :

$$(\Delta Z)_{j+(1/2)}^{n+(1/2)} = V_{j+(1/2)}^{n+(1/2)} [s_1 \dot{\epsilon}_1 + (d-1) s_2 \dot{\epsilon}_2]_{j+(1/2)}^{n+(1/2)} \Delta t^{n+(1/2)} ,$$

where

$$s_1^{n+(1/2)} = \frac{1}{2} (s_1^{n+1} + s_1^n), \text{ etc.}$$

Total internal energy, E:

$$(E)_{j+(1/2)}^{n+1} = \left(\frac{E^n - \{(1/2) [A(\eta^{n+1}) + P^n] + \bar{q}\} [V^{n+1} - V^n] + \Delta Z}{1 + (1/2) [B(\eta^{n+1})] [V^{n+1} - V^n]} \right)_{j+(1/2)}$$

where

$$\bar{q} = (1/2) [q^{n+(1/2)} + q^{n-(1/2)}].$$

This equation assumes that the EOS has the form

$$P = A(\eta) + B(\eta)E.$$

In most practical calculations, iteration is required in the routine to obtain both energy and pressure.

Stress and Failure Calculation

Calculate μ , the shear modulus ($\mu \rightarrow 0$ as material melts or if it spalls).

Stress deviators:

$$(s_1)_{j+(1/2)}^{n+1} = (s_1)_{j+(1/2)}^n + 2\mu \left\{ (\dot{\epsilon}_1)_{j+(1/2)}^{n+(1/2)} \Delta t^{n+(1/2)} - \frac{1}{3} \left[\frac{V^{n+1} - V^n}{V^{n+(1/2)}} \right]_{j+(1/2)} \right\}$$

$$(s_2)_{j+(1/2)}^{n+1} = (s_2)_{j+(1/2)}^n + 2\mu \left\{ (\dot{\epsilon}_2)_{j+(1/2)}^{n+(1/2)} \Delta t^{n+(1/2)} - \frac{1}{3} \left[\frac{V^{n+1} - V^n}{V^{n+(1/2)}} \right]_{j+(1/2)} \right\}$$

$$(s_3)_{j+(1/2)}^{n+1} = -[(s_1)_{j+(1/2)}^{n+1} + (s_2)_{j+(1/2)}^{n+1}]$$

$$\sqrt{(s_1^2 + s_2^2 + s_3^2) / (2/3)} = \tau_{\text{oct}} \quad \text{octahedral shear stress}$$

If $\tau_{\text{oct}} \leq Y2F$, the material is within the elastic limit. If not, the material is failing. If the material is failing, determine the new rubble fraction RUBF(P). Then, calculate the new failure surface value of τ_o , $Y2F = \text{RUBF} * Y2FRUB + (1 - \text{RUBF}) Y2FCON$. Y2FRUB and Y2FCON are the rubble and consolidated failure surfaces, respectively.

If the material is failing, use DUCF (the fraction of failure that is ductile rather than brittle) to relax the stresses.

$$\tau_{\text{oct}} = \text{DUCF } Y2F + (1 - \text{DUCF}) \left(\tau_{\text{oct}} - \dot{\gamma} \mu \Delta t - \frac{\mu}{\eta} [\tau_{\text{oct}} - Y2F] \Delta t \right)$$

$\dot{\gamma}$ is a relaxation rate constant of a dislocation type.

η is a viscous constant for a Maxwell solid-like relaxation model.

However, do not permit τ_{oct} to become smaller than $Y2F$. Likewise, relax the pressure, if necessary.

Test to see if the spall condition has been met. If it has, set a sentinel to skip the EOS routine.

Stability

$$\Delta t^{n+(3/2)} = \frac{2}{3} \cdot \frac{\Delta r^{n+1}}{\sqrt{a^2 + b^2}} \Bigg|_{\text{min over } j}$$

$$\Delta r^{n+1} = r_{j+1}^{n+1} - r_j^{n+1},$$

where

a = sound speed

$b = 8 C_0^2 \Delta r^{n+1} (\dot{V}/V)^{n+(1/2)}$

$C_0 = 0$ if $\dot{V}/V \geq 0$.

If $\Delta t^{n+(3/2)} > (1.4) \Delta t^{n+(1/2)}$, use $\Delta t^{n+(3/2)} = (1.4) \Delta t^{n+(1/2)}$.

$$\Delta t^{n+1} = \frac{1}{2} [\Delta t^{n+(3/2)} + \Delta t^{n+(1/2)}].$$

LOGICAL STRUCTURE OF UKO; CODE BLOCKS, SUBROUTINES, AND THEIR PURPOSES

MAIN

A01 MAKE DROP FILE, CLEAR LARGE CORE COMMON. ALSO INCLUDES
COMMON AND MOST DATA STATEMENTS IN A CLICHE.

GENERATOR (SEGMENT 1)

B01 INITIALIZE, READ INPUT TO FIRST END CARD
B05 INVERT INPUT ARRAYS, INITIALIZE, READ REST OF INPUT
B10 FINISH INITIALIZATION

PHYSICS (SEGMENT 2)

C01 EXECUTIVE ROUTINE FOR CYCLE CALCULATIONS. THIS ROUTINE
CALLS SUBROUTINES C05 THROUGH C45, IN THAT ORDER, EACH
CYCLE. ALSO PUNCHES INPUT CARDS.

C05 REZONE

C10 COMPUTE TOTAL STRESSES, BOUNDARY PRESSURE, ACCELERATION

C15 COMPUTE VELOCITY AND RADIUS

C20 COMPUTE STRAIN, VOLUME, Q

C25 CALL EOS, COMPUTE SOUND SPEED SQUARED

C30 COMPUTE STRESS, FAILURE, RELAXATION

C35 COMPUTE ENERGY SUMS AND ENERGY CHECK

C40 PREPARE FOR PLOTS, TEST FOR EDIT OR STOP

C45 COMPUTE DELTA T

D10 EOS 10-19 NOTE -

D20 EOS 20-29 NOT

D50 EOS 50-59 ALL OF

D60 EOS 60-69 THESE

D70 EOS 70-79 EQUATIONS OF

D80 EOS 80-89 STATE ARE

D91 EOS 91-99 PRESENT

OUTPUT (OVERLAY)

E01 EDIT

E05 EXIT

E10 PLOT RADIUS VS. TIME, Q

E15 PLOT P+Q VS. TIME

E20 PLOT VARIOUS FUNCTIONS VS. RADIUS

E25 PLOT RADIAL STRESS VS. TIME

E30 PLOT ENERGY ACROSS REGION BOUNDARY VS. TIME

E35 PLOT DEVIATORS, ETA, AND VELOCITY VS. TIME

E40 PLOT RADIUS VS. TIME CONTOURS

E45 PLOT P AND P-DEVIATORS VS. TIME

The difference equations are located in subroutines C10-C35 and C45. They occur there in the order in which they are listed in Section B, Outline of Finite Difference Equations in UKO.

Equations of state are located in subroutines D10-D91. They are represented as polynomials ($P = P(\mu, E)$), ideal gas equations, Tillotson equations, Mie-Grüneisen equations, and others.

LISTING OF SUBROUTINES FOR ARTIFICIAL VISCOSITY AND FAILURE MODEL

```

*      FORTRAN          C20
SUBROUTINE C20          $$$ COMPUTES STRAIN, VOLUME, G          $$$ C20
USE WZCON
IF (NCYCLE .LE. 2) ,20
DO 10 J = 1, JZZ
10 POLD(J) = P(J)
20 HOLDDPA = P(1) * HOLDPB = P(JZZ+1) $$$ SAVE BOUNDARY PRESSURES
P(1) = P(2) * P(JZZ+1) = P(JZZ) $$$ SET BOUNDARY CONDITIONS
TEMV = 0.          $$$ SET TEMV, TEMVA FOR
TEMVA = .083333333333 * DTO * DTO $$$ VOLUME CALC.
J = 1
DO 130 K=1,NR          $$$ BEGIN LOOP OVER ALL REGIONS
NES = NEQST(K)
LK = J + NZR(K) - 1
DO 120 J = J,LK          $$$ BEGIN LOOP OVER ALL ZONES OF A REGION
EOLD(J+1) = E(J+1)
Q(J+1) = 0.
OLDV = V(J+1)
DELU = U(J) - U(J+1)          $$$ VELOCITY STRAINS S1D, S2D
QDIVU = ABSF(-DELU + QM10 * (U(J+1) + U(J)) * (X(J+1) - X(J))
1 * (D - 1.) / (X(J+1) + X(J)))
S1D(J+1) = ( U(J) - U(J+1) ) / ( XXN2(J) - XXN2(J+1) )
S2D(J+1) = 0.
IF (ND .GE. 2) S2D(J+1) = (U(J)+U(J+1))/(XXN2(J)+XXN2(J+1))
GO TO (4C,60,50), ND
40 V(J+1) = V(J+1) + DTO / W(J+1) * RZ(J+1) * DELU          $$$ VOLUME
GO TO 80
50 TEMV = TEMVA * (U(J)**3 - U(J+1)**3)
60 V(J+1) = V(J+1) + DTO / W(J+1) * RZ(J+1) * ( U(J) * XXN2(J)
1 **ND - U(J+1) * XXN2(J+1)**ND + TEMV )
80 VVN2(J+1) = ( V(J+1) + CLDV )*.5
IF (V(J+1) .LE. 0.) 140,
DV(J+1) = V(J+1) - CLDV
DELU = ABSF(DELU)
QRHD = RZ(J+1) / VVN2(J+1)          $$$ DENSITY
SNDCSP = SWRTF(MAX1E(SS(J+1), 1,E-8))          $$$ SOUND SPEED
QDELPA = .5 * (ABSF(P(J+1) - P(J)) + ABSF(P(J+1) - P(J+2)))
TYM = ABSF((X(J+1) - X(J)) / (SNDCSP * DTO))
QDELR = ABSF(TYM * DV(J+1) / RZ(J+1))
IF (QM8 .GT. .5) QDELPA = ABSF(PCLD(J+1) - P(J+1)) * TYM
POLD(J+1) = P(J+1)
DELUW2 = SWRTF(QDELPA * QDELR)
IF (QM9 .GT. .5) QDIVU = .5 * ABSF(QBJ(J) + QBJ(J+1) + G + E) *
1 DTO * TYM
DUQ = QDIVU**QM38 * DELLC2**QM39 * DELU**(1. - QM38 - QM39)
QML1 = QM1(K)
QML2 = QM2(K)
IF (HEAL(J+1) .LT. .9) ,90
QML1 = QML2 * (1. - HEAL(J+1)) * QM1(K)
QML2 = QML2 * (1. - HEAL(J+1)) * QM2(K)
IF (DV(J+1) .GT. 0.) ,100
QML1 = -QML1
QML2 = -QML2
GO TO 100
90 IF (DV(J+1) .GT. 0.) ,100
    
```

QML1 = -CML1 * CM16
 QML2 = -CML2 * CM16

C
 C LINEAR Q FIRST TERM VON NEUMANN, SECOND TERM WHITE \$\$\$ C20
 C LINEAR Q = QM * RHC * DELU * SCUNC SPEED
 C

100 Q(J+1) = SNDSP * QRHO * (CML1 * DELU + CML2 * DUQ)
 IF (DV(J+1) .GE. 0.) 110,

C
 C QUADRATIC Q FIRST TERM VON NEUMANN, SECOND TERM WHITE
 C QUADRATIC Q = QM * RHC * (DELU)**2
 C

Q(J+1) = Q(J+1) + QRHC * (QM3(K) * DELU * DELU + CM4(K) *
 1 DUQ * DUQ)

110 IF (ABSF(Q(J+1)) .LT. QCUT) Q(J+1) = 0.

TESTQ = QM30 * P(J+1)

IF (ABSF(Q(J+1)) .LT. TESTQ) Q(J+1) = 0.

120 CONTINUE \$\$\$ END ZONE LOOP

130 CONTINUE \$\$\$ END REGION LOOP

P(1) = HCLDPA \$ P(JZZ+1) = HCLDPB \$\$\$ RESTORE BOUNDARY PRESSURE
 RETURN

140 JOUT = JZZ-J \$\$\$ ERRCR DETECTED

NOT 59,150 ,JOUT,TIME,NCYCLE

NOT 3, 150 ,JOUT,TIME,NCYCLE

PRINT 150 ,JOUT,TIME,NCYCLE

\$\$\$ C20

JBAD = 1 \$ NEND = 4 \$ CALL C40A

15. FORMAT (1/40H ERROR VOLUME NEGATIVE OR ZERO IN ZONE, 14,4X,1HT,

1 E10.3,4H C,15)

END

```

*      FORTRAN          C30
SUBROUTINE C30      $$$ STRESS, FAILURE, RELAXATION
USE WZCON
J = 1
DO 340 K = 1, NR
    IES = 1
    NES = NEGST(K)
    LK = J + NZR(K) - 1
    DO 330 J = J, LK
        $$$ BEGIN LOOP OVER ALL REGIONS
        $$$ INITIALIZE PRESSURE INDEX
        OLOS1 = S1(J+1)
        OLOS2 = S2(J+1)
        $$$ BEGIN LCOP OVER ZONES OF A REGION
        $$$ SAVE OLD DEVIATORS FOR
        $$$ ELASTIC ENERGY CALCULATION
        DELIAV = .333333333333 * DV(J+1) / VVN2(J+1)

C      IF MATERIAL IS HYDRODYNAMIC, SKIP STRESS DEVIATORS, STRENGTH
C      AND FAILURE
C      IF (STRONG(NES) .EQ. 0.) 320,

C      BEGIN STRESS DEVIATOR, STRENGTH AND FAILURE CALCULATION
C      COMPARE ZONE PRESSURE P(J+1) WITH STRENGTH-RELATED PRESSURES
C      EUSA TO GET INTERPOLATION INDEX IES
C      250 IF (EUSA(IES,NES) .LE. P(J+1)) 260,
        IES = IES + 1
        GO TO 250
C      260 IF (EUSA(IES+1,NES) .GT. P(J+1)) 270,
        IES = IES + 1
        GO TO 250

C      COMPUTE PRESSURE PEM (P SUB M) BETWEEN PEMC (CONSOLIDATED) AND
C      PEMR (RUBBLE) PRESSURES, WHERE STRENGTH CURVE DROPS TO ZERO.
C      270 PEM(J+1) = PEMC(NES) + (PEMR(NES) - PEMC(NES)) * RUBF(J+1)
        EM = 1.
        IF (P(J+1) .LT. 0.) GO TO 275
        EM = (PJOIN(NES) - P(J+1)) / PJOIN(NES)
        IF (P(J+1) .GT. PJOIN(NES)) EM = 0.
        $$$ C30

C      COMPUTE INTERPOLATION FRACTION (PFRAC) FOR CALCULATION OF
C      PRESSURE DEPENDENT FUNCTIONS
C      275 PFRAC = (P(J+1) - EUSA(IES,NES)) / (EUSA(IES+1,NES) - EUSA(IES,NES))

C      FOR ELASTIC MATERIAL WITHOUT FAILURE, INTERPOLATE SHEAR MODULUS
C      AND COMPUTE STRESS DEVIATORS, THEN SKIP STRENGTH AND FAILURE
C      IF (STRONG(NES) .LT. 0.) ,271
        SHRMOD(J+1) = EOSHITES(NES) + (EOSHITES+1,NES) - EOSHITES(NES))
        * PFRAC
        S1(J+1) = S1(J+1) + 2. * SHRMOD(J+1) * (S1D(J+1) * DTO - DELTAV)
        S2(J+1) = S2(J+1) + 2. * SHRMOD(J+1) * (S2D(J+1) * DTO - DELTAV)
        GO TO 320

C      COMPUTE INTERPOLATION FRACTIONS FOR CONSOL. AND RUBBLE CURVES

```

```

C
271 PFRAC = PFRAC + EM * (PEMC(NES) - PEM(J+1))   $$$ CONSOLIDATED
    PFRACR = PFRAC + EM * (PEMR(NES) - PEM(J+1))   $$$ RUBBLE
C
C      SET MELT MULTIPLIER (SMELT) TO ZERO IF ZONE HAS MELTED
C      OR TO A FRACTION IF ZONE IS NEARLY MELTED
C
    SMELT(J+1) = 1.
    EPERGM = E(J+1) * V(J+1) / RR(K)
    IF (EPERGM .GT. EFRAC(NES)) ,277
    IF (EPERGM .LT. EMELT(NES)) ,276
    SMELT(J+1) = (EMELT(NES) - EPERGM) / (EMELT(NES) - EFRAC(NES))
    GO TO 277
276 SMELT(J+1) = 0.
C
C      INTERPOLATE DUCTILE FRACTION (DUCF), A PRESSURE FUNCTION
C
277 DUCF(J+1) = EOSJ(IES,NES) + (ECSJ(IES+1,NES) - EOSJ(IES,NES)) * PFRAC
C
C      COMPUTE HEAL, A MEASURE OF THE HEALING THAT HAS OCCURRED AFTER
C      SPALL
C
    IF (SKPEOS(J+1) .EQ. 1.) ,278
    HEAL(J+1) = 0.
    GO TO 279
278 IF (DUCF(J+1) .GT. DFHEL1(NES)) ,279
    IF (DUCF(J+1) .LT. DFHEL2(NES)) ,A278
    HELLO = ABSF((DUCF(J+1) - DFHEL1(NES)) / (DFHEL2(NES) -
1      DFHEL1(NES)))
    HEAL(J+1) = MAX(HEAL(J+1), HELLO)
    GO TO 279
A278 HEAL(J+1) = 1.
C
C      INTERPOLATE SHEAR MODULUS (SHRMD), A PRESSURE FUNCTION
C      IF ZONE IS MELTED, SMELT = 0.
C      IF ZONE IS NOW SPALLED, (1.-SKPEOS) = 0.
C      IF ZONE IS NOW SPALLED, OR HAS NOT COMPLETELY HEALED AFTER
C      SPALL, HEAL IS LESS THAN ONE.
C      (1.-Y2COEF*Y2SR) MAKES SHEAR MODULUS DEPENDENT ON SHEAR STRESS.
C      SHR MOD PRIME IS USED TO RELAX DEVIATORS AFTER FAILURE.
C      SHR MOD IS USED TO COMPUTE DEVIATORS BEFORE FAILURE, AND
C      SOUND SPEED.
C
279 SHRMPR = (FOSH(IES,NES) + (EOSH(IES+1,NES) - EOSH(IES,NES)) * PFRAC
1 ) * SMELT(J+1) * (1. - Y2COEF(NES) * Y2SR(J+1))
    SHRMOD(J+1) = SHRMPR * HEAL(J+1)
C
C      COMPUTE STRESS DEVIATORS S1, S2, S3
C
    S1(J+1) = S1(J+1) + 2. * SHRMOD(J+1) * (S1D(J+1) * DTC - DELTAV)
    S2(J+1) = S2(J+1) + 2. * SHRMOD(J+1) * (S2D(J+1) * DTC - DELTAV)
    S3 = - S1(J+1) - S2(J+1)
C
C      STORE STRESSES AND PRESSURE FOR POSSIBLE LATER USE IN
C      CORRECTING OVER-RELAXATION.

```

```

C      S1INT = S1(J+1) * S2INT = S2(J+1) * PINT = P(J+1)
C
C      COMPUTE SQUARE ROOT OF I2D (Y2SR)
C
C      Y2SR(J+1) = .81649658 * SQRT( (.5 * (S1(J+1)**2 + S2(J+1)**2
1      + S3**2))
C
C      COMPUTE CUBE ROOT OF I3D (Y3CR)
C
C      SPRDU = S1(J+1) * S2(J+1) * S3
C      Y3CR = SIGN( ((ABS( SPRCG)**.33333333, SPRCG)
C
C      COMPUTE FAILURE SURFACE INTERPOLATION COEFFICIENTS
C
C      CONAA = CONA(IES,NES) + (CONA(IES+1,NES) - CONA(IES,NES)) * PFRACC
C      CONBB = CONB(IES,NES) + (CONB(IES+1,NES) - CONB(IES,NES)) * PFRACC
C      RUBAA = RUBA(IES,NES) + (RUBA(IES+1,NES) - RUBA(IES,NES)) * PFRACR
C      RUBBB = RUBB(IES,NES) + (RUBB(IES+1,NES) - RUBB(IES,NES)) * PFRACR
C
C      COMPUTE FAILURE SURFACE (Y2F)
C      IF ZONE IS MELTED, SMELT = 0.
C      IF ZONE IS NOW SPALLED, OR HAS NOT COMPLETELY HEALED AFTER
C      SPALL, HEAL IS LESS THAN ONE.
C
C      Y2F = ((1. - RUBF(J+1)) * (CONAA + CONBB * Y3CR) + RUBF(J+1) *
1      (RUBAA + RUBBB * Y3CR)) * SMELT(J+1) * HEAL(J+1)
C
C      IF ZONE HAS SPALLED SKIP FAILURE TEST AND REDUCE DEVIATORS.
C
C      JFAIL(J+1) = 0
C      IF (V(J+1) .GT. VEM(J+1)) 201,
C
C      TEST FOR FAILURE
C
C      IF (Y2F .LT. Y2SR(J+1)) .300
C
C      FAILURE IS OCCURRING IN THIS ZONE THIS CYCLE
C
C      JFAIL(J+1) = 1
C
C      INTERPOLATE EQUILIBRIUM RUBBLE FRACTION (RUBFE) AND LET
C      RUBBLE FRACTION (RUBF) REACH IT IN A SERIES OF STEPS.
C
C      201 RUBFE = EOS1(IES,NES)+(EOS1(IES+1,NES)-EOS1(IES,NES))*PFRAC
C      RUBF(J+1) = RUBF(J+1) + (RUBFE - RUBF(J+1)) * RLXFRG
C
C      COMPUTE LOCATION OF NEW FAILURE SURFACE AFTER FAILURE
C      TO DETERMINE LOWER LIMIT ON RELAXATION IN THIS FAILURE.
C
C      Y2F = ((1. - RUBF(J+1)) * (CONAA + CONBB * Y3CR) + RUBF(J+1) *
1      (RUBAA + RUBBB * Y3CR)) * SMELT(J+1) * HEAL(J+1)
C
C      RELAX STRESS DEVIATORS, SET THEM TO ZERO IF THEY CHANGE SIGN.
C      PART OF THE RELAXATION IS BRITTLE, PART IS DUCTILE.

```


C

REDUCL = SIGSS = 0.

\$\$\$ C30

IF (Y2SR(J+1) .NE. 0.) ,282

REDUCE = Y2F / Y2SR(J+1)

SIGSS = 1. / (ABSF(S1(J+1)) + ABSF(S2(J+1)))

282 AB = REDUCE * DUCF(J+1) + 1. - DUCF(J+1)

CD = (1. - DUCF(J+1)) * CTO * SHRMPR * SIGSS * (3. * EOSY(INE) +

1 (1. - REDUCE) * EOSZ(INE) * Y2SR(J+1))

IF (S1(J+1) .EQ. 0.) ,283

SIHN = 1. * SIHN = SIGNF (SIHN, S1(J+1))

CD1 = CD * ABSF(S1(J+1))

IF (CD1 .GT. FRACSTR(INE)) CD1 = FRACSTR(INE)

S1(J+1) = S1(J+1) * AB - CD1 * SIHN

IF (S1(J+1) * SIHN .LT. 0.) S1(J+1) = 0.

283 IF (S2(J+1) .EQ. 0.) ,284

SIHN = 1. * SIHN = SIGNF (SIHN, S2(J+1))

CD2 = CD * ABSF(S2(J+1))

IF (CD2 .GT. FRACSTR(INE)) CD2 = FRACSTR(INE)

S2(J+1) = S2(J+1) * AB - CD2 * SIHN

IF (S2(J+1) * SIHN .LT. 0.) S2(J+1) = 0.

C

RELAX PRESSURE, SET IT TO ZERO IF IT CHANGES SIGN

C

C

284 IF (P(J+1) .EQ. 0.) ,285

\$\$\$ C30

SIHN = 1. * SIHN = SIGNF (SIHN, P(J+1))

CD = (1. - DUCF(J+1)) * CTO * SHRMPR

DP = EOSL(INE) * CD * (3. * ECSY(INE) + ABSF(P(J+1)) * EOSZ(INE))

IF (P(J+1) .GT. 0.) DP = -CD * CM27

P(J+1) = DUCF(J+1) * P(J+1) + (1. - DUCF(J+1)) * (P(J+1) + DP)

IF (P(J+1) * SIHN .LT. 0.) P(J+1) = 0.

C

C

C

C

C

IF FAILURE IS ENTIRELY DUCTILE (STRESS DOES NOT GO ABOVE
FAILURE SURFACE IN COMPETENT MATERIAL), SET PRESSURE AND STRESS
TO ZERO IN A SPALLED ZONE AS SOON AS IT SPALLS, INSTEAD OF
RELAXING THEM GRADUALLY.

C

IF ((DUCF(J+1) .GT. .99) .AND. (SKPECS(J+1) .EQ. 1.))

1 P(J+1) = S1(J+1) = S2(J+1) = S3 = 0.

C

C

C

C

TEST FOR CVER-RELAXATION AND ADJUST DEVIATORS AND PRESSURE
IF NEEDED.

IF (P(J+1) .GT. 0.) ,285

S3 = -S1(J+1) - S2(J+1)

Y2SRN = .81649658 * SQRTF (1.5 * (S1(J+1)**2 + S2(J+1)**2 + S3**2))

IF (Y2SRN .LT. Y2F) ,285

FRCINT = ABSF(Y2SR(J+1) - Y2F) / ABSF(Y2SR(J+1) - Y2SRN)

S1(J+1) = S1INT + FRCINT * (S1(J+1) - S1INT)

S2(J+1) = S2INT + FRCINT * (S2(J+1) - S2INT)

P(J+1) = PINT + FRCINT * (P(J+1) - PINT)

\$\$\$ C30

C

C

C

COMPUTE RELAXED STRESS AFTER FAILURE, USING RELAXED DEVIATORS

285 S3 = -S1(J+1) - S2(J+1)

Y2SR(J+1) = .81649658 * SQRTF (1.5 * (S1(J+1)**2 + S2(J+1)**2

```

1          + S3**21)
C
C      COMPUTE SPALL PRESSURE PEM AND CORRESPONDING SPALL VOLUME VEM.
C
      PEM(J+1) = PEMC(NES) + (PEMR(NES) - PEMC(NES)) * RUBF(J+1)
288 IF (EOSA(IES,NES) .LE. PEM(J+1)) 289,
      IES = IES - 1
      GO TO 288
289 IF (EOSA(IES+1,NES) .GT. PEM(J+1)) 290,
      IES = IES + 1
      GO TO 288
290 VEM(J+1) = ECSE(IES,NES) + (EOSE(IES+1,NES) - EOSE(IES,NES)) *
1 (PEM(J+1) - EOSA(IES,NES)) / (EOSA(IES+1,NES) - EOSA(IES,NES))
2 + 1.E-100)
      VEM(J+1) = VEM(J+1) / (1. + AMUPZ(NES) * AMUMAX(J+1) / AMUJN(NES))
C
C      SET SKIP-EOS SENTINEL IF ZONE VOLUME V IS GREATER THAN SPALL
C      VOLUME VEM. THIS SENTINEL MAY BE SET THIS CYCLE EVEN IF
C      FAILURE DID NOT OCCUR THIS CYCLE, BECAUSE VEM WOULD HAVE BEEN
C      COMPUTED IN ANY PREVIOUS CYCLE IN WHICH FAILURE OCCURRED.
C
300 SKPEUS(J+1) = 0.
      IF (V(J+1) .GT. VEM(J+1)) ,310          $$$ C30
      IF (P(J+1) .GT. 0.) P(J+1) = 0.
      SKPEUS(J+1) = 1.          $$$ SPALL HAS OCCURRED
C
C      COMPUTE NEW SHEAR MODULUS AFTER FAILURE
C
310 SHRMUL(J+1) = (EOSH(IES,NES) + (ECSH(IES+1,NES) - EOSH(IES,NES))
1 * VFRAC) * SMELT(J+1) * (1. - SKPEUS(J+1)) * HEAL(J+1)
C
C      END OF STRENGTH, FAILURE, RELAXATION CALCULATION
C
320 VDT = .5 * VVN2(J+1) * CTO
      E1(J+1) = VDT * (S1(J+1) + QLOD1) * S1D(J+1)          $$$ ELASTIC ENERGY
      E2(J+1) = VDT * (S2(J+1) + QLOD2) * S2D(J+1) * DC
      E1T(J+1) = E1T(J+1) + E1(J+1)
      E2T(J+1) = E2T(J+1) + E2(J+1)
      E(J+1) = EOLD(J+1) - .5 * DV(J+1) * (P(J+1) + POLD(J+1) + QQ(J+1)
1 + Q(J+1)) + E1(J+1) + E2(J+1)
330 CONTINUE          $$$ END ZONE LOOP
340 CONTINUE          $$$ END REGION LOOP
      RETURN          $$$ C30
      END

```

GLOSSARY OF NAMES IN SUBROUTINES C20 AND C30

CONAIP,EOS)	FAILURE SURFACE COEFFS. OF CONSOLIDATED STRENGTH CURVES AT INPUT VALUES OF STRENGTH CURVES.
CONAA	FAILURE SURFACE INTERPOLATION COEFFICIENTS OF CONSOLIDATED STRENGTH CURVES (EOSB, EOSC) INTERPOLATED BETWEEN INPUT VALUES OF STRENGTH CURVES.
CONB(P,EOS)	FAILURE SURFACE COEFFS. OF CONSOLIDATED STRENGTH CURVES AT INPUT VALUES OF STRENGTH CURVES.
CONBB	FAILURE SURFACE INTERPOLATION COEFFICIENTS OF CONSOLIDATED STRENGTH CURVES (EOSB, ECSC) INTERPOLATED BETWEEN INPUT VALUES OF STRENGTH CURVES.
D	1. PLANE, 2. CYLINDER, 3. SPHERE
DD	0. PLANE, 1. CYLINDER, 2. SPHERE
DELU	SPATIAL VELOCITY DIFFERENCE.
DELUQ2	SQUARE ROOT OF ((DELTA P * DELTA X * DELTA (1/RHC)) / (SCUND SPEED * DELTA T)) IN Q CALC.
DFHEAL	THRESHOLD VALUE OF DUCTILE FRACTION AT WHICH RECOMPACTION BEGINS TO HEAL A SPALLED ZONE. AT THIS VALUE OF DUCTILE FRACTION THE SHEAR MODULUS OF THE SPALLED ZONE BEGINS TO RETURN FROM ZERO TO ITS NORMAL VALUE. SHEAR MODULUS WILL REACH ITS NORMAL VALUE WHEN DUCTILE FRACTION REACHES 1. OPTIONAL INPUT. DEFAULT = .5
DP	PRESSURE CHANGE IN RELAXING IN BRITTLE FAILURE, A FUNCTION OF SHEAR MODULUS SHMPR, DISLOCATION MODEL FAILURE RATE EOSY, AND RECIPROCAL OF MAXWELL VISCOSITY EOSZ.
DT0	DELTA T (TIME STEP) AT THIS CYCLE.
DUCF	DUCTILE FAILURE FRACTION, THE FRACTION OF FAILURE WHICH IS DUCTILE RATHER THAN BRITTLE. A PRESSURE FUNCTION.
DUQQQQ	(DIV U)**QM38 * DELLQ2**QM39 * DELTAU**((1-QM38-QM39) IN Q CALC
DV(J+1)	(VIN+1)-VIN) FOR ZONE J+1/2
E	SPECIFIC INTERNAL ENERGY OF ZONE.
EOLD	SPECIFIC INTERNAL ENERGY OF ZONE IN PREVIOUS CYCLE.
EFRAC(EOS)	FRACTION USED IN MELT TEST. IN INPUT, EFRAC IS A PURE NUMBER (DEFAULT = .8). IN GENERATOR, EFRAC BECOMES A FRACTIONAL PART OF THE MELT ENERGY (EFRAC = EFRAC * EMELT). SEE EMELT.
EM	A FRACTION USED IN INTERPOLATING FAILURE SURFACE COEFFICIENTS.
EMELT(EOS)	MELT ENERGY (PER GRAM) OF A MATERIAL, THE ENERGY REQUIRED TO RAISE TEMPERATURE TO MELTING POINT, PLUS HEAT OF FUSION. USED TO DECIDE WHETHER A ZONE HAS MELTED. DEFAULT = 1.E10
EOSA(EOS)	PRESSURE TABLE FOR STRENGTH, FAILURE, AND RELAXATION CALC.
EOSB(P,EOS)	CONSOLIDATED COMPRESSIVE STRENGTH CURVE.
EOSF(P,EOS)	ORIGINAL VOLUME CURVE (LOADING CURVE).
EOSH(P,EOS)	SHEAR MODULUS.
EOSI(P,EOS)	RUBBLE CURVE FRACTION, THE FRACTION OF THE COMPOSITE STRENGTH CURVE WHICH IS MADE UP OF THE (INPUT) RUBBLE STRENGTH CURVE RATHER THAN THE (INPUT) CONSOLIDATED STRENGTH CURVE.
EOSJ(P,EOS)	DUCTILE (VON MISES) FAILURE FRACTION, THE FRACTION OF FAILURE WHICH IS DUCTILE RATHER THAN BRITTLE.
EOSU(EOS)	PRESSURE RELAXATION MULTIPLIER. DEFAULT = 1.
EOSY(EOS)	DISLOCATION MODEL (BRITTLE) FAILURE RATE, GAMMA DOT. DEFAULT = 1.E10

EOS2(EOS)	RECIPROCAL OF MAXWELL VISCOSITY, $1/\eta$, USED IN RELAXATION AFTER BRITTLE FAILURE.
EPERGM	ENERGY PER GRAM IN A ZONE, USED IN MELT TEST.
E1(J)	ELASTIC ENERGY OF ZONE (RADIAL DIRECTION) ADDED THIS CYCLE.
E1T(J)	ELASTIC ENERGY OF ZONE (RADIAL DIRECTION) SUMMED OVER TIME.
E2(J)	ELASTIC ENERGY OF ZONE (TANGENTIAL DIRECTION) ADDED THIS CYCLE
E2T(J)	ELASTIC ENERGY OF ZONE (TANGENTIAL DIRECTION) SUMMED OVER TIME
FRACSTR	FRACTION OF MAX. OF CONSOLIDATED COMPRESSIVE STRENGTH CURVE (EOSB). SEE EOST.
FRGINT	A RATIO OF STRESS DIFFERENCES, USED IN RECALCULATING OVER-RELAXED STRESSES AND PRESSURE AFTER FAILURE
HOLDPA	TEMPORARY STORAGE FOR OUTER BOUNDARY PRESSURE IN THIS ROUTINE
HOLDPB	TEMPORARY STORAGE FOR INNER BOUNDARY PRESSURE IN THIS ROUTINE
IES	INDEX OF PRESSURE TABLE (EOSA)
J	INDEX OF ZONES AND ZONE INTERFACES
K	INDEX OF REGIONS
LK	NO. OF ZONES IN THIS REGION
MU	$(1-V)/V$, WHERE V IS RELATIVE SPECIFIC VOLUME
MUJOIN	MU VALUE AT WHICH LOADING AND UNLOADING P VS. MU CURVES JOIN.
MUMAX	MINIMUM OF (MAX. MU EVER REACHED BY THIS ZONE, OR MUJOIN)
MUPZ	MU AT FOOT OF UNLOADING P VS. MU CURVE.
NCYCLE	CYCLE NUMBER OF PROBLEM.
ND	1 PLANE , 2 CYLINDER , 3 SPHERE
NDO	0 PLANE , 1 CYLINDER , 2 SPHERE
NEQST(K)	EOS OF REGION
NES	EQUATION OF STATE OF CURRENT REGION
NR	NUMBER OF REGIONS TO BE CALCULATED THIS CYCLE
NZR(K)	NUMBER OF ZONES IN REGION K
OLDV	RELATIVE SPECIFIC VOLUME AT LAST PREVIOUS CYCLE.
P	PRESSURE IN ZONE THIS CYCLE
PEM	PRESSURE AT WHICH STRENGTH CURVE OF THIS ZONE THIS CYCLE INTERSECTS PRESSURE AXIS - THAT IS, PRESSURE AT WHICH STRENGTH GOES TO ZERO. THE STRENGTH CURVE WILL BE SOME COMBINATION OF THE INPUT CONSOLIDATED STRENGTH CURVE AND THE INPUT RUBBLE STRENGTH CURVE, SO PEM WILL COINCIDE WITH PEMC OR PEMR OR LIE BETWEEN THEM.
PEMC	PRESSURE (P SUB M, CONSOLIDATED) IN PRESSURE TABLE (EOSA) CORRESPONDING TO LAST ZERO VALUE IN CONSOL. COMPRESSIVE STRENGTH CURVE (EOSB) - PRESSURE AT WHICH CONSOLIDATED COMPRESSIVE STRENGTH CURVE DRIPS TO ZERO.
PEMR	PRESSURE (P SUB M, RUBBLE) IN PRESSURE TABLE (EOSA) CORRESPONDING TO LAST ZERO VALUE IN RUBBLE COMPRESSIVE STRENGTH CURVE (EOSD) - PRESSURE AT WHICH RUBBLE COMPRESSIVE STRENGTH CURVE DRIPS TO ZERO.
PFRAC	RATIO OF PRESSURE DIFFERENCES, USED TO INTERPOLATE VARIOUS FUNCTIONS OF PRESSURE SUCH AS STRENGTH AND SHEAR MODULUS.
PFRACC	MODIFIED FORM OF PFRAC, USED TO INTERPOLATE CONSOLIDATED STRENGTH.
PFRACR	MODIFIED FORM OF PFRAC, USED TO INTERPOLATE RUBBLE STRENGTH.
PINT	TEMPORARY STORAGE FOR PRESSURE JUST BEFORE FAILURE CALC. IT MAY BE USED AFTER FAILURE TO RECALCULATE AN OVER-RELAXED PRESSURE.
PJOIN	PRESSURE IN EOSA TABLE AT WHICH CONSOL. AND RUBBLE COMPRESSIVE STRENGTH CURVES BECOME EQUAL
POLD	PRESSURE IN ZONE AT LAST PREVIOUS CYCLE

Q(J)	ARTIFICIAL VISCOSITY IN ZONE J-1/2
QBJ(J)	ACCELERATION OF INTERFACE J
QCUT	MIN. OF ABSOLUTE VALUE OF Q ALLOWED. DEFAULT = 1.E-10 A Q SMALLER THAN THIS WILL BE SET TO ZERO AS SOON AS IT IS COMPUTED.
QDIVU	DIVERGENCE OF U (VELOCITY), USED IN Q CALC.
QML1	COEFFICIENT OF VON NEUMANN TERM IN LINEAR Q.
QML2	COEFFICIENT OF WHITE TERM IN LINEAR Q.
QM1	A FACTOR IN QML1, THE COEFF. OF VON NEUMANN TERM IN LINEAR Q. OPTIONAL INPUT. DEFAULT = 0.
QM2	A FACTOR IN QML2, COEFF. OF WHITE TERM IN LINEAR Q. OPTIONAL INPUT. DEFAULT = .1
QM3	COEFFICIENT OF VON NEUMANN TERM IN QUADRATIC Q. OPTIONAL INPUT. DEFAULT = 0.
QM4	COEFFICIENT OF WHITE TERM IN QUADRATIC Q. OPTIONAL INPUT. DEFAULT = 3.
QM8	SENTINEL IN Q CALC. IF GREATER THAN .5, IT WILL CAUSE RECALCULATION OF QQDELP. OPTIONAL INPUT. DEFAULT = 0.
QM9	SENTINEL IN Q CALC. IF GREATER THAN .5, IT WILL CAUSE RECALCULATION OF QDIVU (DIVERGENCE OF VELOCITY). OPTIONAL INPUT. DEFAULT = 0.
QM10	COEFFICIENT IN QDIVU (DIVERGENCE OF VELOCITY) CALC. OPTIONAL INPUT. DEFAULT = 1.
QM12	FACTOR IN COEFFICIENT OF VON NEUMANN AND WHITE TERMS IN LINEAR Q. USED ONLY WHEN ZONE IS SPALLED OR WHEN IT HAS NOT HEALED COMPLETELY AFTER A SPALL. OPTIONAL INPUT. DEFAULT = 5.
QM16	FACTOR IN COEFFICIENT OF VON NEUMANN AND WHITE TERMS IN LINEAR Q. USED ONLY WHEN ZONE IS EXPANDING AND IS NEITHER SPALLED NOR HEALING. OPTIONAL INPUT. DEFAULT = 2.
QM30	COEFFICIENT OF ZONE PRESSURE IN Q CUTOFF TEST. OPTIONAL INPUT. DEFAULT = .002 SEE TESTC.
QM38	EXPONENT IN WHITE TERM IN QUADRATIC Q. OPTIONAL INPUT. DEFAULT = .54
QM39	EXPONENT IN WHITE TERM IN QUADRATIC Q. OPTIONAL INPUT. DEFAULT = .45
QM27	COEFFICIENT OF PRESSURE CHANGE IN RELAXATION AFTER BRITTLE FAILURE. USED ONLY WHEN PRESSURE IS GREATER THAN ZERO. (SEE OP) OPTIONAL INPUT. DEFAULT = 0.
QQ	Q FROM LAST PREVIOUS CYCLE.
QQDELP	DELTA PRESSURE (SPATIAL DIFFERENCE) IN Q CALC.
QQDELR	$\Delta T(X) * \Delta T(1/RHO) / (SCUND SPEED * \Delta T)$ IN Q CALC.
QQQRHO	PRESENT DENSITY OF ZONE IN Q CALC.
REDUCE	FAILURE STRESS Y2F DIVIDED BY APPLIED STRESS Y2SR. USED TO CALCULATE STRESS DEVIATOR RELAXATION AFTER FAILURE.
RLXFRC	RELAXATION FRACTION, A COEFFICIENT IN CALC. OF RUBBLE FRACTION. CAN BE USED TO LET RUBBLE FRACTION REACH ITS EQUILIBRIUM VALUE OVER AN EXTENDED TIME. OPTIONAL INPUT. DEFAULT = 1.
RUBFE	EQUILIBRIUM VALUE OF RUBBLE FRACTION. SEE RLXFRC.
RZ	REFERENCE DENSITY OF ZONE.
SHRMOD	SHEAR MODULUS. USED TO COMPUTE DEVIATORS BEFORE FAILURE, AND SOUND SPEED.
SHRMPR	SHEAR MODULUS PRIME. SIMILAR TO SHRMOD BUT IS UNAFFECTED BY SPALL OR HEALING AFTER SPALL. USED TO RELAX DEVIATORS

SIGNF	AFTER FAILURE. SIGN FUNCTION. SUPPOSE $A = \text{SIGNF}(B,C)$ THEN A WILL HAVE THE MAGNITUDE OF B AND THE SIGN OF C.
SIHN	TEMPORARY STORAGE FOR THE ALGEBRAIC SIGN OF VARIOUS QUANTITIES
SNOSPD	SOUND SPEED
SPLSEN	SPALL SENTINEL, A FRACTION. $(1-\text{SPLSEN})$ MULTIPLIES THE SHEAR MODULUS AND IS A MEASURE OF THE HEALING THAT HAS OCCURRED AFTER SPALL. WHEN SPLSEN IS GREATER THAN .1, THE LINEAR Q COEFFICIENT IS INCREASED TO REDUCE THE NOISE INHERENT IN THE RECOMPACTION OF SPALLED MATERIAL.
SS	SOUND SPEED SQUARED
STRFRM	A FRACTION (ZERO TO ONE, INCLUSIVE) WHICH IS A MEASURE OF THE COMPETENCE OF THE ZONE. = 0. WHEN ZONE IS SPALLED. = 1. WHEN ZONE HAS NOT SPALLED OR HAS COMPLETELY HEALED AFTER SPALL.
S1	USED TO MULTIPLY SHEAR MODULUS AND STRENGTH.
S1D	RADIAL STRESS DEVIATOR
S1INT	RADIAL STRAIN RATE TEMPORARY STORAGE FOR RADIAL STRESS DEVIATOR S1, COMPUTED JUST BEFORE FAILURE CALC. MAY BE USED AFTER FAILURE CALC. FOR RECALCULATION OF OVER-RELAXED STRESS.
S2	TANGENTIAL STRESS DEVIATOR
S2D	TANGENTIAL STRAIN RATE
S2INT	TEMPORARY STORAGE FOR TANGENTIAL STRESS DEVIATOR S2, COMPUTED JUST BEFORE FAILURE CALC. MAY BE USED AFTER FAILURE CALC. FOR RECALCULATION OF OVER-RELAXED STRESS.
S3	THIRD STRESS DEVIATOR
TESTQ	A FRACTION OF THE ZONE PRESSURE. Q IS SET TO ZERO AS SOON AS COMPUTED IF ITS ABSOLUTE VALUE IS LESS THAN THIS. COEFFICIENT OF PRESSURE FOR THIS TEST IS QM30, AN OPTIONAL INPUT NUMBER. DEFAULT = .002
TIME	PROBLEM TIME AT END OF THIS CYCLE IN MICROSECONDS.
TYMMMM	PART OF THE WHITE TERM IN LINEAR AND QUADRATIC Q CALC.
V(J)	RELATIVE SPECIFIC VOLUME ($\text{RHOZERC}/\text{RHO}$) AT WHOLE CYCLE.
VEM(J)	RELATIVE SPECIFIC VOLUME AT WHICH STRENGTH OF MATERIAL IN THIS ZONE GOES TO ZERO. USED TO DECIDE WHETHER ZONE IS SPALLED. IF VOLUME OF ZONE IS GREATER THAN VEM, ZONE MUST BE SPALLED AND SPALL SENTINEL SKPEOS IS SET. NOTE - HYDRODYNAMIC MATERIAL IS NEVER ALLOWED TO SPALL.
VVN2(J)	RELATIVE SPECIFIC VOLUME ($\text{RHOZERC}/\text{RHO}$) AT HALF CYCLE.
W(J)	MASS OF ZONE PER RADIAN OR STERADIAN.
WZCON	NAME OF CLICHE STATEMENT CONTAINING COMMON AND DATA STATEMENTS
X(J)	POSITION OF ZONE BOUNDARY AT WHOLE CYCLE.
XXN2(J)	POSITION OF ZONE BOUNDARY AT HALF CYCLE
Y2COEFF	Coefficient WHICH CAN BE USED TO MAKE SHEAR MODULUS DEPENDENT ON SHEAR STRESS. $(1-\text{Y2COEFF})$ MULTIPLIES THE SHEAR STRESS. OPTIONAL INPUT. DEFAULT = 0.
Y2F	STRENGTH OF MATERIAL IN THIS ZONE THIS CYCLE - A POINT ON THE FAILURE SURFACE OF MATERIAL IN THIS ZONE. IT IS COMPARED WITH APPLIED STRESS Y2SR TO DECIDE WHETHER ZONE IS FAILING. IF ZONE FAILS, Y2F IS RECOMPUTED WITH THE AFTER-FAILURE RUBBLE FRACTION AND COMPARED WITH AFTER-FAILURE VALUE OF APPLIED STRESS Y2SRN TO DETERMINE WHETHER STRESSES WERE OVER-RELAXED IN FAILURE.

Y2SR APPLIED STRESS IN THIS ZONE THIS CYCLE - SQUARE ROOT OF I2D.
 IT IS COMPARED WITH STRENGTH Y2F TO DECIDE WHETHER ZONE IS
 FAILING.

Y2SRN APPLIED STRESS IN THIS ZONE AFTER FAILURE HAS OCCURRED THIS
 CYCLE AND STRESSES HAVE BEEN RELAXED. IT IS COMPARED WITH
 AFTER-FAILURE STRENGTH TO DETERMINE WHETHER STRESSES WERE
 OVER-RELAXED IN FAILURE.

Y3CR CUBE ROOT OF I3D, AN INVARIANT FUNCTION OF STRESS DEVIATORS
 AND ONE OF THE COORDINATE AXES OF THE FAILURE SPACE.

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Appendix:

UKO Example Calculation (Pre-Schooner II)

It should be noted that the one-dimensional (spherical) UKO calculations reported here can be compared to the experiment only with respect to the spall velocity at ground zero (GZ). After spallation begins, the field experiment becomes two dimensional.

$P - \mu$ (pressure vs $\mu = (1 - V)/V$, where V is relative specific volume) data are given in Fig. A-1. These data were obtained from the vitrophyre sample 2 on page 2 of Ref. 12. This material is appropriate for use as an average medium for a depth of

Fig. A-1. P vs μ for Pre-Schooner II.

burial of 21.65 m. We make no attempt to mock-up the many layers of geologic material at the site; these layers are described in Chapter 5 of Ref. 13, and from this source we also obtain the remainder of the material properties of the rock. From Table 5.1 and Fig. 5.1 of Ref. 13, we obtain an average density of 2.33 g/cc, an average compressive strength of 5 kbar, and an average shear modulus of 0.2 Mbar. We arbitrarily set the failure surface as in Fig. A-2 by using the above compressive strength and

by using the Schooner data¹⁴ as a guide, since the two types of rock are not too dissimilar. The region of the failure surface below a pressure of 6 kbar is most important, since only a small portion of the material experiences larger pressures, i.e., it is most important that the slope of the τ_o (octahedral shear stress) - P curves be approximately correct.

Fig. A-2. Failure surface for Pre-Schooner II. The same curves are used for extension and compression.

The material is ductile above 6-kbar pressure and is brittle below 2 kbar, with a smooth linear transition between. For failure at negative pressure, the new surface is given by the rubble surface; and, for failure above 6-kbar pressure, the failure surface is given by the consolidated surface. These two surfaces are mixed linearly between these two values.

The high-explosive (HE) used to create the crater was nitromethane (NM), which is a fluid and can be easily poured into a preformed chamber. NM has a density of 1.13 g/cc and an energy content of 1200 cal/g. For the experiment, a spherical chamber had been prepared whose volume was to hold 100 tons of NM with its center at a depth of 21.6 m. However, some of the explosive leaked, and the shot was fired with only 86% of the volume occupied. The actual chamber volume was used in the UKO calculation, but the HE density was put at 0.97 g/cc. A standard KO (No. 1) EOS for HE was used, with its energy per unit mass modified to the NM value. The HE chamber and emplacement description can be found in Ref. 15.

The camera used to record surface motion at GZ exposed slightly less than one frame per msec, and this low resolution was degraded further by the smoothing techniques necessary to perform the data analysis. Pictures were taken of a large (4 X 16 ft) plywood target mounted on a heavy 6-in. o.d. pipe set in concrete, so the target was very inert and poorly coupled to the earth; these difficulties made it virtually impossible to resolve the acceleration details of the earth during the spall phase. However, if a state of dynamic equilibrium (plywood target and earth at the same constant velocity) is reached and maintained sufficiently long, then the spall velocity should be measurable. From Fig. 4.2 of Ref. 15, the displacement-vs-time

data from 30 to 70 msec appear to fit this criterion quite well, so one obtains a spall velocity of 3.9 cm/msec to within an accuracy of about 3%.

Three calculations were run on UKO with various zone sizes so that the effect of artificial viscosity could be estimated and eliminated. The coarsely zoned problem had six zones in the HE (~46 cm each) and 45 zones in the rock (~43 cm each). The spall velocity of the outermost 43-cm section was 3.12 cm/msec. Another problem was run in which each of the above zones was halved, and the outermost 43 cm of rock experienced a spall velocity of 3.52 cm/msec. Each zone was halved once more for the third calculation, and the outermost 43-cm section spalled at a velocity of 3.76 cm/msec. These spall velocities can be plotted as a function of relative zone size, and a curve can be extrapolated to zero zone size. The extrapolated spall velocity is approximately 4.0 cm/msec, compared with 3.9 from the experiment. The actual geologic materials are quite inhomogeneous, the EOS's of the rock samples that were measured are quite crude, and the numerical model is quite simplistic. When these factors are considered, the agreement is considerably within that which would be considered satisfactory.

The P-V data can be considered to be fairly reliable, even though the measurements are static. One might, however, expect the failure surfaces to change noticeably as the strain rates change. A similar calculational series was run (varying zone size) with the ductile strength raised by 50%, and the resulting spall velocity was reduced by only 10%.

Figures A-3 through A-8 show stress and velocity as a function of radius at various times, for the fine-zone calculation of Pre-Schooner II. The first two of these figures show the system when the shock is approaching the free surface. Note that the pressure is not continuous across the HE-rock interface, because of the presence of shear modulus in the rock. The rarefaction is accompanied by spallation in Figs. A-7 and A-8. Figure A-8 specifically shows the velocity increase at the rarefaction front.

After the rarefaction has reached the cavity, the HE gas begins to recompact the spalled material; and the spalled material and the gas-acceleration phase begins, in which a second push of the material is accomplished. The actual recompaction process is quite two dimensional and is included here only to demonstrate code behavior for a portion of the rock mechanics model that is quite difficult to handle. Note that the recompaction process involves a discontinuity in the material behavior, i.e., material at zero pressure (no matter what density) is suddenly changed to a material for which the EOS must be used. A large linear q is used to damp out noises at the recompaction front (see Fig. A-7), although some noise remains. In Fig. A-7 we also observe a material quasi-interface that results from the fact that the rock to the right of the quasi-interface has lost its elastic properties as a result of the spallation process, and the pressure has not become large enough to heal the material. This last feature of the calculation is a result of the specific way in which the UKO model allows spalled material to heal. Even though this part of the model is considered experimental, examination of Fig. A-8 shows that the solution is well behaved. It should be added

Fig. A-3. Stress profiles for the diverging wave. Time = 3.0 msec at Cycle 507.

that the energy conservation is excellent; the energy content of the problem changes by less than 0.01% when the problem goes from cycle 507 to cycle 1683 (Figs. A-3 to A-8).

Fig. A-4. Velocity profiles for the diverging wave. Time = 3.0 msec at Cycle 507.

Fig. A-5. Stress profile for the rarefaction wave. Time = 7.0 msec at Cycle 922.

Fig. A-6. Velocity profile for the rarefaction wave. Time = 7.0 msec at Cycle 922.

Fig. A-7. Stress profile for the recompaction wave. Time = 13.0 msec at Cycle 1683.

Fig. A-8. Velocity profile for the recompaction wave. Time = 13.0 msec at Cycle 1683.

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