**SOC73: A ONE-DIMENSIONAL
WAVE PROPAGATION CODE
FOR ROCK MEDIA**

John F. Schatz

November 5, 1974

MASTER

Prepared for U.S. Atomic Energy Commission under contract No. W-7405-Eng-48

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Printed in the United States of America
Available from

National Technical Information Service
U. S. Department of Commerce

5285 Port Royal Road

Springfield, Virginia 22151

Price: Printed Copy \$ ____*; Microfiche \$1.45

*Pages

1-50
51-150
151-325
326-500
501-1000

NTIS
Selling Price

\$4.00
\$5.45
\$7.60
\$10.60
\$13.60

LAWRENCE LIVERMORE LABORATORY
University of California, Livermore, California, 94550

UCRL-51689

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SOC73, A ONE-DIMENSIONAL WAVE PROPAGATION CODE FOR ROCK MEDIA

Abstract

SOC73 is a highly modified version of SOC, a computer code that numerically simulates mechanical wave propagation in geologic media. Innovation in SOC73 lies mainly in the constitutive modeling of solid media. New models have been introduced in which the pressure-volume behavior and the behavior of brittle, ductile, and tensile failure are more continuous

and representative of laboratory and field observations than before. There are also new methods of low-pass compressional filtering and high-pass distortional filtering that are more physically and numerically satisfying. Finally, the concept of failure-associated strain has been introduced. It allows an estimate of the damage caused to the medium by an inelastic stress wave.

Introduction

The evolution of the computer code SOC, originally conceived by Seidl,¹ has been described by Schatz,² and Cherry and Petersen.³ SOC73 is the latest version of that code and Petersen has written a user's manual for it.⁴ SOC73, like SOC, has been used to numerically calculate one-dimensional, adiabatic, finite-strain, nonlinear mechanical wave propagation in geologic media. As the code evolved, the numerical method (explicit finite difference in a Lagrangian coordinate frame) remained largely unchanged.^{1,3} What we have changed considerably is the constitutive model for solid earth media, where, for our purposes, a constitutive model may be defined as a functional relationship between stresses, strains, and internal energy which describes material behavior. Thus, aside from introductory remarks, this paper will primarily

consider constitutive modeling in SOC73.

Although the solid media constitutive routine in SOC73 is but a portion of the bulk of the code, it represents our knowledge of material behavior. Thus, it is of crucial importance with respect to the outcome of predictive calculations for earth media. The general philosophy of SOC73 constitutive modeling is to make major improvements in SOC written in such a way that further improvements will follow as our knowledge of material behavior increases. Unfortunately, because such knowledge is in a state of flux, it is difficult to produce a "final" report. This means that there are known shortcomings and areas under development in SOC73. These will be noted as they arise.

Throughout this report, vector and tensor notation will be avoided, even though such notation would lead to considerable conciseness. We choose to keep the mathematical notation elementary in order to make the report an introduction to the constitutive physics of SOC73 which may be read by people of virtually any level of mathematical ability.

EQUATIONS OF MOTION AND CONTINUITY

The major task of a code such as SOC73 is to integrate the one-dimensional equation of motion with respect to time, while applying the boundary and initial conditions desired by the user. SOC73 allows planar, cylindrical, and spherical geometries in a Lagrangian coordinate frame. Thus, the equation of motion takes the forms

$$\frac{1}{V} \dot{u}_x = \frac{\partial \sigma_x}{\partial x} + B_x \quad (1)$$

in planar geometry,

$$\frac{1}{V} \dot{u}_r = \frac{\partial \sigma_r}{\partial r} + \frac{1}{r} (\sigma_r - \sigma_\theta) + B_r \quad (2)$$

in cylindrical geometry, and

$$\frac{1}{V} \dot{u}_r = \frac{\partial \sigma_r}{\partial r} + \frac{1}{r} (\sigma_r - \sigma_\theta) + \frac{1}{r} (\sigma_r - \sigma_\phi) + B_r \quad (3)$$

in spherical geometry, where V is the specific volume defined by

$$V = \frac{1}{\rho} \quad (4)$$

A dot indicates time differentiation following a particle path, and x , r , θ , and ϕ are fixed coordinates. In Eqs. (1) through (4), ρ is density, u is velocity, σ is stress (defined as negative in compression) and B is body force. For a planar

problem, the coordinates are x , y , and z , but y and z do not appear; for a cylindrical problem, they are r , θ , and z , but z does not appear; and for a spherical problem they are r , θ , and ϕ , where $\sigma_\theta = \sigma_\phi$. The subscripts indicate components in these coordinate directions. (Equation (3) will be simplified later.)

Figures 1, 2, and 3 show typical problems run in these geometries using SOC73. A typical planar problem is to simulate a plate impact experiment, where a gas gun is used to accelerate a projectile with known properties into a target of unknown properties (Fig. 1). Gauges in the target measure velocity and stress as functions of time and position. When these measurements are combined with calculations, the results can be used to deduce constitutive properties. A typical cylindrical problem is to simulate the detonation of chemical high explosives

Fig. 1. A typical problem in planar geometry, where a flat projectile impacts an unknown target.

in a cylindrical hole (Fig. 2). The calculation is used to predict the extent of rock fracture. A typical spherical problem is to simulate an underground nuclear explosion (Fig. 3). The calculation is used to predict fracture, ground motion, peak stresses, etc.

In SOC73, Eqs. (1) through (3) cannot be used conveniently, so in the following paragraphs we have defined a new stress system. In the laboratory, we often measure constitutive properties in terms

of pressure vs volume and shear stress vs shear strain. Let us then define pressure, P , as the negative mean stress. In planar geometry,

$$P = -\frac{1}{3} (\sigma_x + \sigma_y + \sigma_z), \quad (5)$$

where $\sigma_y = \sigma_z$.

In cylindrical geometry

$$P = -\frac{1}{3} (\sigma_r + \sigma_\theta + \sigma_z), \quad (6)$$

where σ_θ does not, in general, equal σ_z .

In spherical geometry

$$P = -\frac{1}{3} (\sigma_r + \sigma_\theta + \sigma_\phi), \quad (7)$$

where $\sigma_\theta = \sigma_\phi$.

Now, we can use conventional stress deviator terminology to define

$$s_i = P + \sigma_i, \quad (8)$$

where s_i is the i^{th} stress deviator and i is any one of the coordinates x, y, z, r, θ , and ϕ . We may now rewrite the equations of motion as

$$\frac{1}{V} \dot{u}_x = \frac{\partial}{\partial x} (-P + s_x) + B_x \quad (9)$$

in planar geometry.

Fig. 2. A typical problem in cylindrical geometry, where a high explosive charge is detonated in a bore hole.

Fig. 3. A typical problem in spherical geometry, where a nuclear explosive is detonated underground.

In cylindrical geometry

$$\frac{1}{V} \dot{u}_r \approx \frac{\partial}{\partial r} (-P + s_r) + \frac{1}{r} (s_r - s_\theta) + B_r. \quad (10)$$

In spherical geometry

$$\frac{1}{V} \dot{u}_r \approx \frac{\partial}{\partial r} (-P + s_r) + \frac{2}{r} (s_r - s_\theta) + B_r. \quad (11)$$

The four dependent variables in (9) are V , u_x , P , and s_x , and the five in (10) and (11) are V , u_r , P , s_r , and s_θ . To complete the system, we need three more equations in planar, and four more equations in cylindrical and spherical geometries.

One of the necessary equations is the equation of continuity. Because of the time integration in SOC73 it is most convenient to describe continuity in terms of the strain rates $\dot{\epsilon}_i$, or

$$\dot{\epsilon}_x = \frac{\partial u_x}{\partial x} \quad \dot{\epsilon}_y = \dot{\epsilon}_z = 0 \quad (12)$$

in planar geometry.

In cylindrical geometry

$$\dot{\epsilon}_r = \frac{\partial u_r}{\partial r} \quad \dot{\epsilon}_\theta = \frac{u_r}{r} \quad \dot{\epsilon}_z = 0. \quad (13)$$

In spherical geometry

$$\dot{\epsilon}_r = \frac{\partial u_r}{\partial r} \quad \dot{\epsilon}_\theta = \dot{\epsilon}_\phi = \frac{u_r}{r}. \quad (14)$$

Then the substitution of Eqs. (12), (13), or (14) into the equation for volumetric strain rate

$$\frac{\dot{V}}{V} = \sum_{i=1}^3 \dot{\epsilon}_i \quad (15)$$

gives the continuity equation for any coordinate system. We also need two equations for P and s_x in planar geometry and three for P , s_r , and s_θ in cylindrical geometry. These remaining equations

are the so-called constitutive relations. They may or may not be given in closed form, and may or may not be interdependent. In our case, we choose that the constitutive relations be equations of pressure and stress deviators as functions of position, time, strain, strain rate, past history, and perhaps internal energy.

Before considering SOC73 constitutive modeling in detail, we note that SOC73 input and output is not written in terms of deviators, but instead uses a stress quantity, K , defined by

$$K = -\frac{1}{2} (\sigma_x - \sigma_y) \quad (16)$$

in planar geometry, and

$$K = -\frac{1}{2} (\sigma_r - \sigma_\theta) \quad (17)$$

in cylindrical and spherical geometries.

Because σ_x , σ_y , σ_r , and σ_θ are principal stresses, K is the maximum shear stress in planar and spherical geometries. However, in cylindrical geometry, the third stress, σ_z , is not necessarily equal to one of the other two stresses. In this case, K is the maximum shear stress only in the $r - \theta$ plane. SOC73 uses K because experimental measurements are commonly presented in terms of maximum shear stress. With substitution of K , the equation of motion takes the forms

$$\frac{1}{V} \dot{u}_x = -\frac{\partial}{\partial x} (P + \frac{4}{3}K) + B_x \quad (18)$$

In planar geometry,

$$\frac{1}{V} \dot{u}_r = -\frac{\partial}{\partial r} (-P + s_r) - \frac{2}{r} K + B_r \quad (19)$$

in cylindrical geometry, and

$$\frac{1}{V} \dot{u}_r = -\frac{\partial}{\partial r} (P + \frac{4}{3}K) - \frac{4}{r} K + B_r \quad (20)$$

in spherical geometry. To arrive at (18) through (20), we have made use of the fact

that the sum of the stress deviators is zero.

In the remainder of this report we will retain deviator notation. However, to simplify further mathematical manipulation, we will combine the three equations of motion (9), (10), and (11) to give

$$\frac{1}{V} \dot{u}_r = \frac{\partial}{\partial r} (-P + s_r) + \frac{(d-1)}{r} (s_r - s_\theta) + B_r \quad (21)$$

In like manner, the equation of continuity (15) becomes

$$\frac{\dot{V}}{V} = \frac{\partial u_r}{\partial r} + \frac{(d-1)}{r} u_r \quad (22)$$

where $d = 1, 2$, and 3 for planar, cylindrical, and spherical geometries, respectively. The only important change introduced in (21) and (22) is that the planar coordinate is called r instead of x . It will become apparent later that the retention of a simple deviator terminology, as in (21) and (22), rather than the use of K , is desirable for manipulating the code internally.

BODY FORCE

The body force, B_r , appearing in Eq. (21) and in the other equations of motion, is the component of gravity in the r -direction. In a problem with planar geometry, this is easily evaluated by determining the angle of the r -axis with respect to gravity. Unfortunately, in cylindrical or spherical problems, which have a center of symmetry at $r = 0$, the presence of gravity causes an inherent non-one-dimensionality. Nevertheless, we wish to gain some information as to the effect of gravity on such a

problem without having to go to the complexity and time consumption of a two-dimensional code.

Figure 4 shows how SOC73 simulates gravity in the spherical case. First, the user decides on the direction of wave propagation of most interest (usually vertical). Then, SOC73 finds the component of gravity in that direction and assumes that it is a uniform body force in the r -direction, as shown in Fig. 4. This is, of course, inaccurate for any propagation path other than the one chosen. Fortunately, for the chosen path, the error introduced locally in g

Fig. 4. Simulation of gravity as a radial body force in spherical geometry.

is proportional only to the cosine of the angular deviation from that path. Using this method, one can estimate, for example, the nonsphericity of a wavefront under the influence of gravity by running several problems, each with a different angle. The same may be done for the cylindrical case.

BOUNDARY AND INITIAL CONDITIONS

This report is not meant to be a user's manual; nevertheless, it is worthwhile to describe several of the methods of energizing the media for the calculation. Energy is usually deposited at an inner boundary. Outer boundaries are usually assumed to be free surfaces. The options allowed in SOC73 are

- Simulated nuclear explosion

First, the innermost region in the problem is specified as "iron gas" with the appropriate volume and mass of a nuclear device (made to be an equivalent sphere). This volume of gas is given an initial internal energy equal to the yield of the device. The subsequent cavity expansion, vaporization of rock material, and motion are then calculated by the code.

- "Bubble" simulated nuclear explosive

The so-called bubble was developed as a means of approximating the complete problem as described above, but with the use of less computer time. Currently, there is seldom need for the small saving in time, but the bubble is occasionally a simplifying convenience. The bubble assumes that 70 metric tons of rock are vaporized per kiloton of

device yield.⁵ The problem starts with a volume of vaporized rock with that spherical radius beyond which vaporization no longer occurs. This volume contains the energy of the nuclear device distributed uniformly. No iron gas is added because the volume of the rock gas bubble is considerably larger than the volume of the iron in the device. The bubble is only a crude approximation of a true nuclear explosion for regions in the immediate vicinity of the expanding cavity and for times immediately after detonation. However, it fits the data well at times greater than a few microseconds and at a distance greater than a few cavity radii.⁶

- Chemical high explosive (HE)

If a volume of HE material is the SOC73 source of energy, the explosive may be placed anywhere and allowed to yield energy in some finite time (as compared to a nuclear explosion, which is essentially instantaneous). Most problems of this sort are run in cylindrical geometry, to simulate an explosion in an underground bore hole. An appropriate constitutive equation to represent the burn and expansion of the gaseous detonation products must be used.

- Pressure or velocity at a boundary as a function of time

If the pressure vs time at a nuclear or high explosive-caused cavity wall is measured or calculated, an initial peak followed by a more-or-less exponential decay is seen (possibly with some ringing).

It is therefore a sufficient approximation for many problems to use pressure or velocity as a function of time as an internal boundary condition. It certainly saves computer time and eliminates unnecessary complexity. This is often a good way to do a parameter study.

- Velocity or precompression in a region

There are some problems, such as planar projectile impact, that require a mass with a prescribed initial velocity and compression to initiate the motion of a medium.

- Overburden

The overburden effect, or gravitational precompression of a deeply buried geologic material, is also treated as an initial condition in SOC73. It is assumed to have an additive effect on the pressure-volume constitutive model.

GENERAL CONCEPTS OF SOC73 CONSTITUTIVE MODELING

The remainder of this paper will consider the SOC73 constitutive models in detail. Both the theory and the necessary user input to the code will be discussed. We will follow a progression of ideas from the simplest, namely elasticity, to the most current, nonlinear, nonelastic model. This approach is convenient in that it is also a roughly historical treatment of the development of the code. We will begin with nonrate-dependent models, which saw the earliest development, and finish with the current rate-dependent modifications. Wavefront damping, which is needed to prevent nonphysical oscilla-

tions, will be treated as a rate-dependent constitutive relation.

Most of SOC73's constitutive models are in the form of stress-strain relationships and do not include the effect of internal energy. However, if the modeled media melts or vaporizes and expands, the effect of internal energy is added. The use of stress-strain alone for the modeling of solids is a convenience justified by the supposition that shock-induced heating is of little importance in the majority of geologic wave propagation problems.

The differential equations that SOC73 integrates, and their finite difference approximations, assume homogeneous, isotropic, and continuous material properties. This means that the user will have a problem if he wants properties that vary rapidly as functions of space or time. Usually, the problem of rapid time variation is solved by internally adjusting the finite integration time step; however, it is impossible to entirely prevent the user from introducing rapid variations, via the constitutive relations, that would tax SOC73's ability to produce an accurate, stable solution. An example of a difficult problem area involving rapid variation is the impingement of a shock wave on a material interface with strong property differences across that interface. It would be best to write special boundary equations in this case. But, as a matter of fact, we depend on the code's built-in viscous damping alone to reduce the magnitude of boundary error. Most remaining rapid variation difficulties are produced by a shock-caused change in material properties that effectively produces a moving material boundary. In fact, almost all rapid variation problems may

be thought of as boundary problems. SOC73's solutions to these problems will

be included in the remainder of this report.

Rate Independent Constitutive Models*

HOOKE'S LAW: LINEAR ELASTICITY

The simplest constitutive relationship that could be used in SOC73 is linear elasticity, or Hooke's law, which states that there is a linear relationship between stress and strain. However, the discrete time integration in the code makes it more convenient to express the law in terms of stress rates and strain rates:

$$\dot{\mathbf{p}} = -k \frac{\dot{V}}{V} \quad (23)$$

$$\dot{\mathbf{s}}_i = 2G \left(\dot{\epsilon}_i - \frac{1}{3} \frac{\dot{V}}{V} \right), \quad (24)$$

where $\dot{\mathbf{s}}_i$ is the i^{th} stress deviator given by Eq. (8), $\dot{\epsilon}_i$ is the i^{th} strain rate given by Eqs. (12), (13), and (14), and $\dot{V}/V$ is the volumetric strain rate given by Eq. (15). The parameters k and G are the elastic bulk modulus and shear modulus, respectively. Remember that two constitutive equations are required for planar geometry, and three for cylindrical and spherical. Equation (23) always provides one of these. Equation (24), for planar geometry, takes the form

$$\dot{s}_r = \frac{4}{3} G \frac{\partial u_r}{\partial r} \quad (25)$$

so that the complete set comprises Eqs. (9), (15), (23), and (25). For cylindrical geometry, we have

$$\dot{s}_r = \frac{2}{3} G \left(2 \frac{\partial u_r}{\partial r} - \frac{u_r}{r} \right) \quad (26)$$

and

$$\dot{s}_\theta = -\frac{2}{3} G \left(\frac{\partial u_r}{\partial r} - 2 \frac{u_r}{r} \right) \quad (27)$$

so that the complete set comprises Eqs. (10), (15), (23), (26), and (27). For spherical geometry,

$$\dot{s}_r = \frac{4}{3} G \left(\frac{\partial u_r}{\partial r} - \frac{u_r}{r} \right) \quad (28)$$

and

$$\dot{s}_\theta = \dot{s}_\phi = -\frac{2}{3} G \left(\frac{\partial u_r}{\partial r} - \frac{u_r}{r} \right) \quad (29)$$

so that the complete set comprises Eqs. (11), (15), (23), (28), and (29).

INCREMENTAL ELASTICITY

Unfortunately, real materials under large stresses and strains can seldom be described by two constant moduli of linear elasticity. Figures 5 and 6 demonstrate this fact by comparing the behavior predicted by Hooke's law to the actual behavior measured in the laboratory for a granodiorite.⁷ The obvious differences shown in the figures imply that SOC73 cannot, in general, use Eqs. (23) or (24) only.

For pressure-volume behavior, probably the simplest modification to the law of linear elasticity would be to assume that behavior is linear for any small increment

*The following sections pertain to solid material only, unless otherwise noted.

Fig. 5. Pressure-volume behavior of a granodiorite. The solid line fits the data⁷; the dashed line is Hooke's law for $k = 400$ kbar.

Fig. 6. Shear stress-shear strain behavior of a granodiorite⁷. The solid line fits the data⁷; the dashed line is Hooke's law for $G = 270$ kbar.

of pressure change, and that k is a function of pressure. Then, because SOC73 integrates stepwise through time, and solves for velocity and strain at each time step, we can replace Eq. (23) with

$$\dot{P} = -k(P) \frac{\dot{V}}{V}, \quad (30)$$

where $k(P)$ is a function given by the user. In SOC73, this function is defined by a tabulation of μ vs P where μ is a measure of the volume given by

$$\mu = \frac{V_0 - V}{V}, \quad (31)$$

where V_0 is the initial specific volume, and V is the deformed volume. The "P- μ table" is usually obtained from hydrostatic pressure-volume measurements.

To find the bulk modulus, we use the relation

$$k(P) = \frac{\partial P}{\partial \mu} (\mu + 1). \quad (32)$$

One then may use the P- μ table and Eqs. (32) and (30) to calculate pressure-volume behavior. However, if the code user has provided a P- μ table, then the pressure-volume relationship at any point may be found by simply looking up the table. SOC73 uses such a table look-up and interpolation, and Eq. (30) is only used to help determine the unloading behavior of porous material (to be discussed in the next section).

For shear stress-shear strain behavior, we might expect to use an equivalent model, namely a shear strain-dependent shear modulus. However, unless rock failure has occurred, we use a simpler model. That is, the user assumes either that the shear modulus, G , is constant, using Eq. (24) directly, or that Poisson's ratio, ν , is constant. If ν is constant, then G is

given from elastic theory by

$$G(P) = \frac{3}{2} k(P) \left(\frac{1 - 2\nu}{1 + \nu} \right). \quad (33)$$

For porous rocks, a constant ν is usually a better choice than a constant G , at least up to the point of failure. All other variations in shear behavior are taken into account later as part of shear failure modeling.

To see why a constant ν is desirable for porous material, note that it implies that G is proportional to k . Thus, when porous material "crushes" and the bulk modulus, in effect, becomes small, the shear modulus also becomes small. This is consistent with the concept, presented below, that shear and volumetric failure are closely related. On the other hand, if we assume a constant G , then Eq. (33) might require a negative Poisson's ratio for small k . This would probably occur early in a loading cycle, before the onset of shear failure. In spherical and cylindrical calculations, test problems have shown that this initiates an ingoing collapse at the front of an outgoing compressional wave, a physically unrealistic situation.

PRESSURE-VOLUME HYSTERESIS

A striking and important example of failure occurs in the pressure-volume behavior of many porous materials. (Failure is here defined as the inability of a material to continue supporting any or all the stresses applied to it.) Whereas hard, nonporous rocks have essentially repeatable pressure-volume behavior for many cycles of loading and unloading, porous geologic materials show a pronounced hysteresis and permanent set,

as demonstrated by the data for a tuff⁸ shown in Fig. 7. This is best attributed to the phenomena of irreversible pore collapse. The most important characteristics of this behavior are:

- A "knee" in the initial, or virgin loading curve, up to which behavior is elastic and beyond which collapse or "crush up" occurs. The knee may be thought of as the onset of volumetric failure.
- A "fully crushed" region, in which it is difficult or impossible to obtain any further irreversible collapse.
- A continuous family of intermediate curves, describing various stages of partial pore collapse.

The basic features of the SOC73 model describing this type of behavior are carried over from SOC, and are shown

Fig. 7. Pressure-mu behavior of a tuff.⁸ The loading curve begins at $\mu = 0$. Two unloading curves are shown, one from 10 kbar and one from 2 kbar.

In Fig. 8. The user provides an initial loading table $\mu(P)$ and a crushed P-mu table, called $\mu_c(P)$. He also specifies μ_1 , the value of μ at which crushing begins. The pressure, P_1 , which corresponds to μ_1 , may be called the "crushing strength." The code then determines μ_2 , the value of μ at which crushing is complete, as the intersection point of $\mu(P)$ and $\mu_c(P)$. For loading or unloading where the maximum μ that has been read ($\mu_{\max}$) is greater than μ_2 , all paths coincide with $\mu_c(P)$. The partial pore collapse model, new to SOC73, is as proposed by Terhune, *et al.*⁹ It is basically an algebraic method of fitting unloading and reloading paths to laboratory data in the partially crushed region and has little justification in terms of physical mechanisms.

Let us call the maximum μ that has been reached $\mu_{\max}$. Then, the partial

Fig. 8. SOC73 pressure-volume loading and unloading model. $\mu(P)$ is the initial loading curve, $\mu_c(P)$ is completely crushed, and $\mu_{pc}(P)$ lies between,

collapse region is defined by the case of $\mu_{\max}$ being greater than μ_1 but less than μ_2 . Assume that μ_r , the points on the $P = 0$ axis to which μ returns after partial crushing, can be specified in the form

$$\mu_r = \mu_c(0)(a_1x + a_2x^2 + a_3x^3), \quad (34)$$

where $\mu_c(0)$ is the value of μ to which a completely crushed material returns; a_1 , a_2 , and a_3 are constants specified by the user; and x is given by

$$x = \frac{\mu_{\max} - \mu_1}{\mu_2 - \mu_1}. \quad (35)$$

The maximum value of x is 1.0, which occurs when $\mu_{\max} = \mu_2$. Note that it is required that $a_1 + a_2 + a_3 = 1.0$. If this were not the case, then complete crushing ($x = 1.0$), would not result in $\mu_r = \mu_c(0)$, and the partially crushed region would not merge continuously into the fully crushed region. Hopefully, the required constants, a_1 , a_2 , and a_3 can be found by a fit to laboratory unloading data. For example, the tuff data shown in Fig. 7 are fit fairly well by $a_1 = 1.08$, $a_2 = -0.55$, and $a_3 = 0.47$. If no such data are available, a reasonable assumption is that $a_1 = 1.0$ and $a_2 = a_3 = 0$, which says that μ_r is essentially spaced in proportion to $\mu_{\max}$ only.

To complete the model, a means of determining the shape of the unloading and reloading paths between $\mu_{\max}$ and μ_r is needed. Call these paths $\mu_{pc}(P)$ and assume that they are given by

$$\mu_{pc}(P) = \mu_c(P) - \mu_e(P) - [\mu_c(P_{\max}) - \mu_{\max}], \quad (36)$$

where $P_{\max}$ is the pressure corresponding

to $\mu_{\max}$ and $\mu_e(P)$ is a pressure-dependent "elastic recovery" of pore space. Assume also that $\mu_e(P)$ is given by the following linear variation with respect to pressure

$$\mu_e(P) = b \left(1 - \frac{P}{P_{\max}} \right), \quad (37)$$

where b is a constant which can be determined from the unloading states μ_r . That is, when $P = 0$, $\mu_{pc}(P)$ must equal μ_r . This results in

$$b = \mu_c(0) - \mu_r - \mu_c(P_{\max}) + \mu_{\max}. \quad (38)$$

If pressure becomes negative, a simple straight line extrapolation of $\mu_{pc}(P)$ is made. Inserting (37) into (36), differentiating, and rearranging terms, we obtain

$$\frac{\partial P}{\partial \mu_{pc}} = \frac{\frac{\partial P}{\partial \mu_c}}{1 + b \frac{\partial P}{\partial \mu_c}}. \quad (39)$$

Equation (39) is then used with (32) and (30) to find the pressure. If $\mu_e(P)$ is relatively small (the usual case), then Eq. (39) produces an unloading curve that is close to a line parallel to the completely crushed curve, as shown schematically in Fig. 8. An example of the behavior produced for tuff by this model has been compared with the experiment (Fig. 9). Also shown is the result of the simplifying assumption that $a_1 = 1$, and $a_2 = a_3 = 0$. This simplification often produces results that are within the range of experimental error.

There is one immediate problem with the partial crushing model as described. If $\mu_e(P)$ is to be an elastic recovery of pore volume, then we would expect it to be positive, which means that b would

also have to be positive. Suppose, however, that the loading and crushed P - μ curves are as shown schematically in Fig. 10. Then, to produce the correct

Fig. 9. SOC73 unloading model applied to tuff.⁸

Fig. 10. Possible anomalous unloading behavior in SOC73 model, shown by dashed line. Dotted line, given by Eq. (40), is used instead.

result at $P = 0$, a negative value of b would be required. Unfortunately, aside from not representing recovered volume, such a condition could cause the unloading curve to have an infinite slope at some point, which is intolerable for reasons of mathematical stability. To counter this possibility, if the "trial" b as calculated from Eq. (38) is negative, the entire P - μ model is replaced by a straight line connecting $\mu_{\max}$ and μ_r :

$$\mu_{pc}(P) = \mu_r + \frac{P}{P_{\max}} (\mu_{\max} - \mu_c) \quad (40)$$

Work is currently proceeding on an improved pore collapse model based on physical mechanisms of deformation.¹⁰

COUPLING OF COMPACTION AND SHEAR

The most severe shortcoming of the SOC73 pressure-volume hysteresis model is that it ignores the effect of deviatoric stress on volume. In Fig. 11, we compare two pressure-volume curves for tuff.⁸ Both are obtained for cylindrical samples, but one is for hydrostatic loading ($\sigma_z = \sigma_\phi = \sigma_r$) and the other is for uniaxial strain loading ($\epsilon_r = \epsilon_\theta = 0$). For hydrostatic loading there is no deviatoric stress, while for uniaxial strain loading there is a finite deviatoric stress. The curves obtained are different. The uniaxial test exhibits "shear enhanced compaction," which means that the material is more compacted at a given pressure than for a hydrostatic test.

In SOC73, the user would most often use the hydrostatically-derived curve for input. Therefore, if the path followed in the calculation were uniaxial instead, a significant error could result. To

counter this, one should probably use as input a curve obtained from a test configuration nearer to the one he wishes to study. Uniaxial strain would be the most appropriate for shock loading. However, changes of configuration during unloading (and the additional existence of rate effects to be discussed later) make the choice of loading curves a complex issue. A better model for SOC73, which is now being developed,¹¹ is a shear strain-volume coupled model of porous material behavior. This model stems from the soil modeling concepts of Schofield and Wroth.¹² The so-called "cap" model¹³ has also stemmed from these concepts. A further advantage of the new model is that dilation, as well as compaction, is accounted for.

EFFECT OF OVERBURDEN

In a calculation, it is often desirable to simulate the effect of being deeply buried in the earth. We take the simple

Fig. 11. Pressure-volume loading behavior for a tuff,⁸ showing the difference between hydrostatic and uniaxial strain loading.

course of assuming that overburden may be treated as an isotropic overpressure which is pre-applied to the material. In this sense, overburden is simply an initial condition of starting at $P = P_0$ instead of $P = 0$. There are, in general, three spherical and one cylindrical overburden possibilities, as shown in Fig. 12. (Planar problems are not usually run with overburden.) In the spherical case, calculations may be horizontal, vertical upward, or vertical downward. Cylindrical calculations are only horizontal.

Fig. 12. Possible configurations for calculations including overburden.

For horizontal calculations, overburden (P_0) is the same for all materials and is specified by the user. For vertical calculations, P_0 varies with depth as

$$P_0(r_0) = \int_0^{r_0} \rho(r) g dr, \quad (41)$$

where r_0 is the initial depth of the calculational zone in question.

We want the initial pressure-volume conditions of the grid to be such that mechanical equilibrium exists; i.e., we do not want gravitational collapse to initiate motion. The simplest way to account for overburden would be to find the pressure and density that correspond to mechanical equilibrium from the user-provided P - μ curves. These points must satisfy Eq. (41). Unfortunately, this simple approach leads to a possible inconsistency for porous material. Suppose that the overburden pressure in a zone is calculated by this procedure, or, as in the horizontal case, is assumed by the user. If this pressure is greater than the pressure P_1 , corresponding to μ_1 (Fig. 13), then problem initiation will occur when the material is in a state of volumetric failure. If P_1 is the equilibrium strength of the porous material, such initiation of failure is unrealistic. Furthermore, it leads to the conclusion that strength is inversely dependent on depth, which is not supported by the laboratory data¹⁴ shown in Fig. 14. In fact, the data in this particular figure would indicate that strength is almost directly proportional to depth. (There is not enough data yet to support a general conclusion.)

The simplest correction of part of this difficulty is to require that all P - μ curves have a large P_1 . This is entirely

Fig. 13. Simplest model for the effect of overburden. It leads to the possibility that $P_0 > \mu_1$.

Fig. 14. Strength of Merlin alluvium as a function of depth.¹⁴ Values have been approximately adjusted to a water content of 10% and a confining pressure proportional to the depth of burial by using, respectively, Figs. 7 and 6 of Ref. 14.

adequate for the horizontal case. In the vertical case, the near-surface zones, with a small overburden, would be unrealistically strong, and strength would still vary inversely with depth. SOC73 corrects this by specifying that loading would always begin at the $P = 0$ point on the P - μ curve. To achieve the (still necessary) equilibrium, we then transform the P and μ coordinates for each zone (Fig. 15). The transformation is given by

$$\begin{aligned}\mu' &= \mu + \mu(P_0) \\ P' &= P + P_0.\end{aligned}\quad (42)$$

In the remainder of this report, we will use unprimed P and μ , and implicitly assume that the transformation given by Eq. (42) has been carried out, if necessary. Note that P must increase an amount $\Delta P = P_1$ before crushing begins, which means that the SOC73 assumption is that crushing of porous material begins

Fig. 15. SOC73 model for effect of overburden. P - μ coordinates for each zone are transformed by P_0 and $\mu(P_0)$.

at a constant value of pressure above overburden. (Strength is unvarying with depth.) For those who disagree with this approach, the old approach is left in the code as an option.

SHEAR FAILURE

Most geologic materials, when subject to an increasing deviatoric stress, eventually stop supporting that stress in an elastic manner. An example is the upper part of the shear stress-shear strain curve shown in Fig. 6. Attempts to explain this type of behavior with a modulus-hysteresis model (like the one we use in P-mu space), though perhaps possible in principle, are not very successful in practice because the paths followed in shear stress-shear strain space are not as simply dependent on stress, strain, and past history as are the P-mu paths. What do we replace Eq. (24) with to account for shear failure?

SOC73 separates shear failure into brittle and ductile regimes. Furthermore, there is no volume dependence in SOC73's shear failure. This lack of volume dependence, a disadvantage mentioned above, nevertheless allows a major simplification. That is, pressure is not affected by shear failure, and the theory can be written entirely in terms of the modification of stress deviators. To model shear failure, we begin by establishing, from triaxial compression test data, a set of failure surfaces in K-P space (Fig. 16). Recall that for the standard cylindrical triaxial test, K is defined by

$$K = \frac{1}{2} (\sigma_z - \sigma_r) \quad (43)$$

where σ_z is the axial (piston) stress and σ_r is the radial (confining) stress. As shown in Fig. 16, the surfaces are actually lines above which a stable state of stress and strain cannot exist. Call them $K_v(P)$ and $K_f(P)$, where v denotes virgin material and f denotes previously failed material. K_f must always be below or identical to K_v .

To make the SOC73 failure routine independent of the coordinate frame, we use stress and strain invariants in our failure theory. (See the article by White.¹⁵) Pressure is already a stress invariant, so we need to find another stress invariant, or a combination of invariants, to represent K. Consider the second and third deviatoric stress invariants:

$$I_{2d} = \frac{1}{6} [(s_1 - s_2)^2 + (s_2 - s_3)^2 + (s_3 - s_1)^2] \quad (44)$$

$$I_{3d} = s_1 s_2 s_3$$

Fig. 16. Failure surfaces for triaxial compression in k-P space, showing virgin curve, failed curve, and brittle-ductile transition.

If we refer to (8), (16), and (17), we obtain

$$\begin{aligned} I_{2d} &= \frac{4}{3} K^2 \\ I_{3d} &= -\frac{16}{27} K^3 \end{aligned} \quad (45)$$

for plane and spherical geometries. For cylindrical geometry, we obtain

$$\begin{aligned} I_{2d} &= -2K^2 + 3K s_z \\ I_{3d} &= 2K^2 s_z + K s_z^2 \end{aligned} \quad (46)$$

because K is defined in the $r-\theta$ plane. The complication of the extra deviator appearing in (46) supports our desire to write the failure model in terms of invariants only, although the use of K is convenient for describing experimental and calculational results.

In an effort to make failure data in triaxial compression consistent with failure data in triaxial extension, as shown by Cherry and Petersen,³ and discussed by Schatz,² we chose to write the failure surfaces in the functional form

$$K = f \left(P + \frac{K}{3} \right). \quad (47)$$

Since failure surfaces in compression and extension are now assumed to coincide, and the sign of K no longer matters, we may write the invariant equivalent of Eq. (47)

$$I_{2d}^{1/2} = f \left[P - \frac{1}{2} \left(\frac{I_{3d}}{2} \right) \right]^{1/3}. \quad (48)$$

Some theoretical justification of Eq. (48) results from the assumption that failure is a two-dimensional process even in a three-dimensional body. We might expect that to be the case if there are only

two different principal stresses, which is probably why Eq. (48) is successful for compression and extension tests. However, there is little theoretical justification for the use of Eq. (48) in a general stress state. Nevertheless, for simplicity and consistency, we use Eq. (48) for all geometries. Therefore, SOC73 rewrites the user's failure surfaces in the form of Eq. (48) by the use of Eq. (45). This is allowed because the required data must be obtained from a test where two principal stresses are equal. The original failure surfaces are thus redefined as

$$I_{2d}^{1/2} = I_v(\bar{P}) \quad (49)$$

$$I_{2d}^{1/2} = I_f(\bar{P}),$$

where v and f denote virgin and failed, respectively, and $\bar{P} = P - \frac{1}{2} \left(\frac{I_{3d}}{2} \right)^{1/3}$.

Now that we have a failure surface description, how does SOC73 execute shear failure? If failure has not occurred, material is assumed to distort elastically. Then, the stress deviators are given by Eq. (24). If, however, loading has proceeded such that the failure surface I_v is exceeded, then stress deviators are reset (or "relaxed") to their value on the I_f surface at the current pressure (Fig. 17). Since we have not changed the pressure, the shear failure procedure is given by

$$s_i' = s_i \frac{I_f}{I_v} \quad (50)$$

for each deviator, where the prime denotes the value after adjustment, and s_i is calculated from (24). If $I_{2d}^{1/2}$ becomes

Fig. 17. SOC73 model for rate-independent shear failure. Dashed lines show loading paths leading to brittle and ductile failure.

less than I_f , then failure ceases, and behavior becomes elastic again.

In the ductile regime, this procedure corresponds to ideal, nonstrain hardening, incompressible plasticity. In the brittle regime, we cannot similarly identify the model, except by pointing out that the decreased strength of the failed material is an attempt to simulate, in a continuum sense, the stress relaxation normally associated with brittle failure.

For materials that exhibit observably plastic macroscopic failure, failure in the ductile regime is probably adequately modeled by the above scheme, although we have not accounted for the often-observed strain hardening. Unfortunately, the brittle failure scheme we have thus far described is inadequate because it is unstable. The numerical reason for instability is easy to see. Brittle failure, as described above, would cause an instantaneous reduction of stress deviators. Such a reduction would induce nonphysical

oscillations in the numerical grid. We must therefore change the brittle failure model so that it makes a more continuous adjustment in stress. Because brittle failure in real materials occurs via crack propagation, and takes a finite time to occur, it is reasonable that our model should allow time for brittle failure. Such changes in the brittle failure routine in SOC73 amount to rate effects in failure, and as such, they will be described later.

TENSILE FAILURE

We define tensile failure as the state in which I_v has been exceeded and any principal stress is tensile. This means that material that has previously failed in shear has no tensile strength. If tensile failure occurs when shear failure is already proceeding, then the two effects are assumed to occur simultaneously and additively. In the case of triaxial test geometry, tension can occur in K-P space as shown in Fig. 18.

The tensile failure model of SOC73 produces relaxation of tensile stress only. SOC73's procedure is to calculate the principal stresses according to the previously mentioned pressure and deviatoric stress models, and then, if $\sigma_i > 0$, set

$$\sigma_i' = 0 \quad (51)$$

where the prime again denotes the adjusted stress. Because tensile relaxation causes the tensile principal stresses to relax while the others remain constant, and shear relaxation causes the shear stress to relax while the pressure remains constant, it is automatically implied that tensile relaxation affects the P - μ

behavior, while shear relaxation does not. For example, consider the case where σ_1 has relaxed in tension, but σ_2 and σ_3 have not. Call the relaxed value after one time step of relaxation σ_1' . Then the tensile relaxed pressure is given by

$$P' = -\frac{1}{3}(\sigma_1' + \sigma_2 + \sigma_3) \quad (52)$$

or, because $\sigma_1' = 0$,

$$P' = P + \frac{1}{3}\sigma_1. \quad (53)$$

Equation (53) shows that during this increment of tensile relaxation, the pressure has increased by an amount

$$\Delta P_t = \frac{1}{3}\sigma_1. \quad (54)$$

It can be shown that, for a constant volume, such tensile relaxation always corresponds to a pressure increase. There is also a corresponding change in the deviators given by

$$\Delta s_1 = -2\Delta P_t \quad (55)$$

$$\Delta s_2 = \Delta s_3 = \Delta P_t.$$

The tensile relaxation of any other principal stress is handled in a like manner. If more than one relaxation is occurring; i.e., several tensile or tensile plus shear, the effects are simply added. For small changes during a time increment, this procedure should be adequate.

Tensile failure always induces a change of pressure above the previously plotted, P-mu curve (Fig. 19). That is, if tensile failure is occurring, a greater volume of material exists than the P-mu curve would predict for a given pressure. This may be physically interpreted as the opening of tensile void

space, or spallation. However, because SOC73's constitutive models represent continua, we do not create any new free surfaces. However, material that has

Fig. 18. Failure surfaces for triaxial compression and extension in k-P space, showing regions of tension.

Fig. 19. Loading, unloading, and reloading in P-mu space, showing deviation from normal behavior due to tensile failure. Flat segment along $P = 0$ represents a change $\Delta\mu_t$.

failed in tension has, in effect, a much reduced bulk modulus.

We must also specify a means of re-loading after tensile failure. Assume, if tensile void space has been opened, that it must be closed before pressure loading can begin again. This means that SOC73 must keep track of the anomalous volume change associated with tensile failure. Let this volume change for small time increments be given by

$$dmu_t = \dot{m}u_t dt. \quad (56)$$

The total change is found by integrating (56) with respect to time. The rate of volume change, $\dot{m}u_t$, can be determined from the relationship

$$\dot{P}_t = \dot{m}u_t \frac{\partial P}{\partial m u}, \quad (57)$$

where $\dot{P}_t$ is the change rate of tensile-created volume and $\partial P / \partial m u$ is the current slope of the P-mu curve without tensile failure. Using (57) in (56) and assuming integration over time, we obtain

$$\Delta m u_t = \frac{\Delta P_t}{\frac{\partial P}{\partial m u}}, \quad (58)$$

where $\partial P / \partial m u$ is constant. Once $\Delta m u_t$ is known, it is easy to require that, upon reloading, no increase in P will be allowed until $\Delta m u_t$ is removed (Fig. 19). In this way, the tensile void closes, or the spalled material reheals. While closure is occurring, the tensile-failed zone acts very compressible, which is entirely appropriate. However, the implied impedance mismatch between zones could cause reflections to occur in the vicinity of the tensile zone. This might be desirable if we wanted to simulate finite void creation and the production

of near-discontinuities. It is undesirable if the material fails in a more continuous manner. Another shortcoming is that we do not account for the "bulking," or permanent increase in the volume of tensile-failed rubble, but this could easily be added by not allowing $\Delta m u_t$ to completely disappear upon reloading. Note that Eqs. (51) through (58) produce the spall effect in the r-direction only as long as the spalled, or tensile, zone does not grow much larger than the adjoining zones. For the θ - and z-directions, the description is always correct, since one-dimensional coding does not allow, by definition, strain discontinuities in these directions.

The tensile failure routine just described suffers from the same potential pitfall as the brittle failure routines in that sudden changes are allowed. For example, if the virgin failure surface is intersected when a large tension already exists, the tensile stress relaxation will be sudden and large. Therefore, the same problem of stability arises as before. Fortunately, the problem can be resolved by a rate-dependent relaxation, to be discussed later.

FAILURE-ASSOCIATED DISTORTIONAL STRAIN

When a material fails, it is convenient to have some measure of the permanent damage done to that material. In the case of simple elastic-plastic constitutive modeling, the total strain can be separated into its elastic and plastic parts, and the plastic part can be called the "damage strain." Because SOC73's failure routines involve brittle, ductile, and tensile aspects, such a simplification

is not made easily, but the same general concepts can be applied as follows: As material deforms, strains are calculated and elastic stresses are found from Eqs. (23) and (24). Furthermore, if shear or tensile failure is occurring, we add the effects of Eqs. (50) and (51). However, even if failure is occurring, we must calculate the elastic increment of stress based on the current value of strain. Then it is easy to calculate the relaxed part of the stress and to associate it with a strain. We call this strain the failure-associated distortional strain, or more briefly, the "failure strain," and denote it by ϵ_f . Only pure shear distortion and shear distortion associated with tensile failure are considered as contributors to failure strain. Permanent volume distortion produced by pressure-volume hysteresis is not considered. This restriction is convenient, but its appropriateness is currently being investigated.

To relate failure strain to invariants we must first consider the stress deviator changes associated with one calculational time step, Δt . The trial deviator value, found from Eq. (24), is

$$s_i = \tilde{s}_i + 2 G \Delta t \left(\dot{\epsilon}_i - \frac{1}{3} \frac{V}{V} \right), \quad (59)$$

where $\tilde{s}_i$ is the old value. If shear failure occurs, a stress adjustment is made, and the final value is determined according to Eq. (50). If we write the adjustment procedure as

$$s_i^f = s_i + \Delta s_i^f, \quad (60)$$

where the superscript f denotes the failure-associated increment, then

$$\Delta s_i^f = s_i \left(\frac{I_f}{I_{2d}^{1/2}} - 1 \right). \quad (61)$$

There is a corresponding change in the second deviatoric stress invariant. If Eq. (61) is combined with (44), we get, after some manipulation,

$$\Delta \left(I_{2d}^{1/2} \right)^f = I_f - I_{2d}^{1/2}, \quad (62)$$

which is a very simple and convenient result in terms of the failure surface I_f and the elastic value of $I_{2d}^{1/2}$. This result should not be surprising, as it is in direct analogy with Eq. (60). Since shear failure is volume independent, we define

$$\Delta \epsilon_f = - \frac{\Delta \left(I_{2d}^{1/2} \right)^f}{2G}, \quad (63)$$

which gives

$$\Delta \epsilon_f = \frac{I_{2d}^{1/2} - I_f}{2G}. \quad (64)$$

Equation (64) is then summed over time (integrated) to give ϵ_f . Because $I_{2d}^{1/2}$ is always greater than I_f when failure occurs, increments of ϵ_f are always positive. That is, when shear failure occurs, positive damage accrues no matter what the direction of the shearing. If the damage is loosely interpreted as uniform motion along a hypothetical crack, then $\Delta \epsilon_f = \Delta L/L$, where L is the length of the crack and ΔL is the motion resulting from shear failure. (Intense but brief failure or weak but persistent failure can produce comparable increases in ϵ_f .) It would be easy to account for strain hardening by using ϵ_f . One could let I_v and I_f grow

as functions of ϵ_f , but this has not been attempted yet.

For tensile failure, the trial deviator value is found from (59). The new value of $\epsilon_d^{1/2}$ after tensile relaxation is calculated and the difference is attributed to the tensile-associated damage. This is then added to ϵ_f using general equation (63).

EXAMPLE OF FAILURE STRAIN: HARDHAT

We have used SOC73 to calculate ϵ_f as a function of radius for the Hardhat 5-kt nuclear explosion in granodiorite. Older SOC calculations for Hardhat that do not include ϵ_f are reported by Cherry and Petersen.² It is most interesting to determine the correlation of ϵ_f with actual fracture density observations. The results of such a correlation are shown in Fig. 20, where we compare the calculated failure-associated strain with several Hardhat failure-indicative observables.¹⁶ From the figure, a consistent pattern seems to emerge:

- The "limit of intense fracture" corresponds to about $\epsilon_f = 0.1 = 10\%$ failure strain.
- The "limit of microscopically detectable fracture" corresponds to about $\epsilon_f = 0.01 = 1\%$.
- The measured chimney height is greater than the limit of the microscopically-detectable fracture and is more nearly equal to the calculated limit of shear failure, which corresponds to $\epsilon_f = 0$.

The above correlations agree within an order of magnitude with laboratory observations of failure in granodiorite,⁷ where a small nonelastic shear strain

(<1%) produces little observable change, while a larger nonelastic strain ($\approx 1\%$) leads to the onset of fracturing. Yet larger nonelastic strains ($\approx 10\%$) usually correspond to complete destruction of the sample. The Hardhat results have interesting implications in terms of predicting permeability enhancement. If we assume that laboratory-detectable microfracture is necessary for any noticeable enhancement of permeability, then we could define the 1% failure strain boundary as the approximate limit of that enhancement. The most severe shortcoming of this method is that we do not use a physical model that explicitly

Fig. 20. Failure-associated strain vs postshot radius for the Hardhat nuclear explosion showing correlation with the microfracture observations of Borg.¹⁶

couples failure strain and permeability. Also, the applicability of the method to highly porous or ductile material has not been investigated.

EFFECT OF LIQUID WATER

The presence of water in the pores of a geologic material has a significant effect on mechanical properties, even if the pressure and temperature are not high enough to induce vaporization or other phase changes. However, because we assume that laboratory measurements are made to determine volume and shear response parameters for SOC73, we do not need to explicitly account for the mechanical effects of water. For example, the apparent weakening in shear of a saturated material is accounted for by the use of a smaller failure envelope, as would be measured in a saturated, undrained test. This procedure is only justified if water is not allowed to move from pore to pore in times comparable to the time of validity for the calculation, but that is usually a safe assumption, as calculations are seldom made for intervals longer than a few tenths of a second.

MODELS INVOLVING INTERNAL ENERGY: LIQUID AND GAS

Most of these models are the same as in SOC,² but we will repeat some of their descriptions here and make a few additions and changes for the sake of clarity. The calculation of internal energy in SOC73 is used explicitly in most of the nonsolid constitutive routines to determine the fluid weighting factor, the melting point, and the vaporization point. In addition to these applications, to be dis-

cussed below, it is used to check consistency. Because the adiabatic process considered can only transfer energy mechanically, the total mechanical energy (internal plus kinetic) must remain equal to whatever energy is given as input to the problem. To calculate the energy, note that the time rate of change of the internal (strain) energy at a point is given by

$$\dot{E} = \sum_{i=1}^3 \sigma_i \dot{\epsilon}_i \quad (65)$$

Equation (65) is used to find the change in internal energy after each time step. To this, we add the kinetic energy, and either divide by the specific volume of a zone to find local energy density, or sum over all zones to find total energy. (We may also add the gravitational potential energy, if necessary.) When a problem is terminated, any discrepancy between the accumulated energy of all the zones and the energy provided by input may be attributed to numerical error.

Consider now the liquid and gaseous models that account for melting, water vaporization, vaporization of solids, and high explosive detonation. By whichever mechanism a material is to approach a fluid state, there must be a way of zeroing the stress deviators, if they were finite prior to the appearance of fluid. (Stress deviators do not exist in an inviscid fluid.) SOC73 achieves the zeroing in a continuous manner by multiplying the strengths, I_f and I_v , by a fluid weighting factor, w_f , given by

$$w_f = \left(\frac{E_f - E}{E_f} \right) \left(\frac{\mu w - \mu}{\mu w} \right) \quad (66)$$

for each zone, where E_f is the specific internal energy for melting (a number provided by the user), E is the calculated internal energy, and μ_w is the compression of the solid necessary to vaporize the contained water (to be discussed below). If there is no water, μ_w is assumed to approach infinity, so that the second factor in (66) approaches unity. Furthermore, we assume that w_t can decrease but not increase, so that it retains its minimum value (but, w_t cannot be less than zero). This corresponds roughly to the physical assumption that loading is adiabatic but unloading is more nearly isothermal. There is usually little effect from the weighting factor, except near to the energy source, and then the effect is primarily numerical smoothing. Therefore, the exact form of Eq. (66) has little physical importance for most rock media problems. The phenomenon of melting is thus treated very simply by SOC73 within the same routine as the constitutive relations for a solid. Melting and subsequent unloading are assumed adiabatic. At each cycle, the internal energy E (per unit volume) of each zone is compared with the melt energy E_f as specified by the user. If E is greater than E_f , then the shear modulus and deviatoric stresses are set to zero. The P - μ curve remains the same as for the solid. If the internal energy drops below the melt energy upon unloading, the zone nevertheless remains liquid because $w_t = 0$.

The concept of melting used by SOC73 follows the reasoning of Butkovich.⁵ When a volume of material is compressed and distorted by a shock wave, and then subsequently unloads, the work done by

the shock loading is not entirely returned to the motion of the material. If this left-over or "waste" energy is assumed to be in the form of heat, and it is sufficiently large, then according to SOC73, it will cause melting. (One could, however, imagine that some of the energy may remain instead as permanent distortion, or as the heat necessary for a solid-solid phase transition, chemical reaction, etc.)

If we deposit enough energy in the material to vaporize water but keep solid material solid, then SOC73 assumes an equilibrium mixture of phases, and allows the water and solid to expand accordingly upon unloading. The adiabatic unloading of such a two-phase system has been calculated by Butkovich.¹⁷ Basically, one combines, by volume weighting, the unloading curves for the solid with the unloading adiabat for water to obtain an unloading curve for the system. In SOC73, the P - V adiabatic release curves for water are stored in the code, and the user only needs to specify the weight fraction of water and the total volumetric strain above which all of the water is assumed to vaporize. For continued loading, the material follows the input P - μ curve, but for unloading, the appropriate expansion adiabat is followed, as shown in Fig. 21. Butkovich has determined that a μ corresponding to a pressure of 100 kbar is a sufficiently good approximation for satisfactory results. Of course, in the actual case, there is a minimum pressure for the onset of vaporization (about 50 kbar) and a maximum pressure for total vaporization (about 700 kbar), and in between, there exists a solid-liquid-gas system.

However, in light of current applications of the SOC73 code, it is not necessary to calculate the complete system.

Solid-solid (or liquid-solid-liquid, etc.) phase changes are not treated explicitly in SOC73, though they can be modeled to some degree by use of P- μ hysteresis. This is a shortcoming. It would be a worthwhile addition to be able to calculate equilibrium and nonequilibrium mixtures of phases.

For the complete vaporization of a solid, or solid-water mixture, we again follow Butkovich.⁵ Basically, the user specifies a vaporization energy E_v which is the internal energy (per unit volume)

Fig. 21. Loading and release paths for Schooner tuff, water, and tuff-water combination.⁵ Dashed curves, identified by primed letters, are for release from 1 mbar.

necessary for complete vaporization. Partially vaporized states are not considered. The value of E_v is at best an educated guess. Butkovich assumes that the "waste heat" necessary to vaporize SiO_2 (the major constituent of most rocks) is 2800 cal/g. If one combines this number with a loading Hugoniot for the solid rock material of interest, he can arrive at the vaporization pressure for that material (Fig. 22). This method, although approximate, is probably as good as possible, given our current

Fig. 22. Shock Hugoniot for granite showing how energy and pressure of vaporization are obtained.⁵ P_v and E_v are determined from $E_v = 1/2 P_v \Delta V/V_0$ when the shaded area is 2800 cal/g.

understanding of the shock vaporization process. Continued loading above the vaporization pressure follows the initial P - μ loading curve. The only problem then is to define the adiabatic unloading curve that the gas follows when it expands.

The gas equation of state, which determines the expansion, is expressed as

$$\gamma - 1 = \frac{PV}{E}, \quad (67)$$

where γ is the effective isentropic or adiabatic exponent. In essence, the gas is treated as ideal for each small increment of unloading. The user has three options. The first two are to provide a table of values of P , E , and ρ or a table of $(\gamma - 1)$, E , and ρ . In either case, since the code at any point has calculated E and ρ , the use of the table and Eq. (67)

will yield the pressure. Butkovich⁵ and Rodean¹⁸ discuss the aptness of the approximations that are involved. The reason for the two-table redundant option is that $(\gamma - 1)$ varies over a much smaller range than P , and the resulting numbers are easier to manipulate. The third option is simply to specify a "short gas table" consisting of one set of P and V values for unloading from the initial density ρ_0 . The validity of the short table depends mostly on the assumption that all vaporized material unloads from a single P - V state at vaporization. This is probably sufficiently accurate for most purposes, but it is seldom necessary to use a short table since complete tables and fast computers are available. A sample P , E , ρ table is shown graphically in Fig. 23.

Fig. 23. Equilibrium gas equation of state for SiO_2 and 1% H_2O by weight.⁵

High explosive detonation is treated basically as a special case of gas expansion; however, due to the finite velocity of detonation, and the complex thermodynamic nature of the expanding gases produced by a high explosive, SOC73 uses a separate routine. Basically, one determines from the detonation velocity and properties of the explosive (as pro-

vided by the user) whether or not burn has occurred in the zone. Several types of explosives can be handled. If burn has occurred, the subsequent adiabatic expansion is determined from a set of tables developed by Lee, *et al.*,^{19,20} or others developed more recently. It does not appear at this point that there are any severe problems with the SOC73 high explosive model.

Rate Dependent Constitutive Models

There are two types of rate dependencies built into SOC73. Both are to some extent necessary for the stability and accuracy of the numerical solution and thus would appear in SOC73 whether or not they were physically necessary. These two mechanisms are Voigt stress relaxation (low-pass filtering), which depends on volumetric strain rate, and Maxwell stress relaxation (high-pass filtering), which depends on shear and/or tensile strain rate. If shock compression and shear or tensile failure are occurring, certain "threshold" values of both damping mechanisms are necessary to the numerical method. However, if the damping terms are allowed to be greater than the threshold values, then they take on a truly physical significance as rate-dependent constitutive terms. The sections below pertain to solid material only.

VOLUMETRIC STRAIN RATE DAMPING

In principle, SOC73 uses the viscosity method²¹ to damp nonphysical grid oscillations. However, the damping term is formulated so that it is not "artificial" as in most wave codes, but "real" in the

physical sense. This statement will be clarified below. Consider the general equation of motion written in terms of principle stresses, and without the body force

$$\frac{1}{V} \dot{u}_r = \frac{\partial \sigma_r}{\partial r} + \frac{d-1}{r} (\sigma_r - \sigma_\theta), \quad (68)$$

where $d = 1, 2$, and 3 for plane, cylindrical, and spherical geometries, respectively. We assume that there is a damping stress, Q , which is subtracted from each of the principle stresses, σ_i , to give an effective principle stress σ_i^*

$$\sigma_i^* = \sigma_i - Q. \quad (69)$$

When changed to pressure and deviator terminology, there results, instead of Eq. (68)

$$\frac{1}{V} \dot{u}_r = -\frac{\partial}{\partial r} (P + Q - s_r) + \frac{d-1}{r} (s_r - s_\theta). \quad (70)$$

The remainder of this discussion is treated more rigorously and in greater detail by Chin²² and Viecelli.²³ I will only outline a few mathematical highlights and discuss the physical principles involved. Note that Q can be thought of as

an effective pressure term. If this term is to modify the driving term of the equation of motion such that there is a resistance to motion; i. e., a viscous damping, then it must be formulated such that a negative velocity gradient produces a positive Q , as shown in Fig. 24. The "standard" linear Q thus has the form

$$Q = -\alpha \rho c \Delta r \frac{\partial u_r}{\partial r}, \quad (71)$$

where c is the speed of sound, α is an adjustable constant, Δr is the zone width, and $\partial u_r / \partial r$ is the velocity gradient. (There is also a "standard" quadratic Q .) The presence of Δr in this expression ensures that Q will disappear as $\Delta r \rightarrow 0$ in the limit of the finite difference approximation. However, this is also what makes Eq. (71) represent an artificial viscosity. The value of such a Q depends strongly on the finite grid spacing. Thus, problems zoned differently, but otherwise physically the same, will still produce different results.

Fig. 24. Schematic diagram of typical shock front, showing dispersive effect of viscosity.

For the solution of the traditional problem of intense shock wave propagation in homogeneous dense materials, the Q formulation of Eq. (71) is desirable. It allows for the damping of oscillations and it can be made arbitrarily small, by reducing zone size or adjusting α , to minimize the physical effect (which is mostly in the form of energy converted from motion to heat). However, waveform data indicate that many, if not most, geologic materials show a strong tendency to cause real, physical damping. It would not be accurate to model such damping with Eq. (71), because real damping should not depend on the grid selection, but only on the material properties. (Also, Eq. (71) was originally intended for plane motion only.)

To obtain the form of the more physically realistic Q used in SOC73, we must replace Δr with a characteristic length, L , for the solid, and make the damping resist volumetric, instead of linear, compression. Consequently, a more appropriate form of Eq. (71) would be

$$Q = -\rho c L \frac{\dot{V}}{V}, \quad (72)$$

where $\dot{V}/V$ is the volumetric strain rate, as found from Eq. (22). For later convenience, we prefer to use a characteristic time, τ_v , rather than length, for damping. Thus, we define

$$L = c \tau_v \quad (73)$$

so that Q , when written out, becomes

$$Q = -\rho c^2 \tau_v \left[\frac{\partial u_r}{\partial r} + (d-1) \frac{u_r}{r} \right]. \quad (74)$$

The planar form of the combination of Eqs. (70) and (74) is called a Voigt viscoelastic solid.²⁴ Such a solid is represented

by a parallel spring and dashpot, and τ_v is called the Voigt relaxation time. The damped motion thus described has the form of a low-pass filter. That is, high frequencies in the wave are preferentially damped, causing the wavefront to spread, or disperse, as it propagates. As time goes on, typical frequencies which characterize the wave front become smaller. If the central frequency in the wave front is assigned a time constant given by its period, τ_s , then at long times, the situation may arise when $\tau_s \gg \tau_v$. If this becomes the case, the wave front will be little further affected by Q . However, if $\tau_s \approx \tau_v$, there will be considerable damping. Thus, the value of τ_v chosen by the user of SOC73 is an important parameter.

In addition to Voigt damping, SOC73 retains a "standard" Von Neumann type quadratic artificial viscosity. We will not discuss it here, because, although necessary, quadratic Q usually has no physical effect on solutions for geologic materials.

CHOOSING THE VOIGT RELAXATION TIME

As mentioned earlier, there is at least a threshold amount of damping of nonphysical oscillations that is required. It is also possible to model physical damping if the real damping properties of the material are so great that the threshold value required is exceeded. To model real, strong damping, we assume that the code user can choose a value of τ_v large enough to match his observed wavelshape. Therefore, what is important at this point is to choose the minimum, or threshold value, correctly. Because the threshold value results from

numerical considerations, we will re-introduce a certain "artificial" zone-size-dependence.

The threshold value of τ_v is determined by that value of Q which is large enough to damp nonphysical grid oscillations. Such oscillations usually occur as overshoot and ringing following the wave front. We must choose the smallest τ_v that will be large enough for numerical damping but not so large that it will disturb the physics. This decision is, of necessity, somewhat subjective because the purpose of each calculation may vary.

Consider the concept of critical (or no overshoot) damping, as shown schematically in Fig. 25. Chin²² shows that critical (or greater) damping in a plane wave front occurs if τ_v is given by

$$\frac{c\tau_v}{\lambda} \geq \frac{1}{2}, \quad (75)$$

where λ is the wavelength in a Fourier decomposition of the wave front. Since the smallest possible wavelength, or the

Fig. 25. Schematic diagrams of shock fronts, showing various degrees of damping.

worst case for oscillation, is given by $\lambda = 2\Delta r$, Eq. (75) is equivalent to

$$\frac{c\tau_v}{\Delta r} \geq 1. \quad (76)$$

Now, consider a wave front that tends to create a moving material discontinuity. It is necessary that damping resist that tendency by smoothing the front so that it contains several grid points. Then derivatives are adequately defined and oscillations are minimized. Our tests have shown that about five zone widths is a reasonable minimum wave front, or "shock width," to satisfy the requirements for both the SOC73 finite difference scheme and for the typical parameter values. What value of τ_v will consistently give a shock width of at least five zones? A study of several problems involving rock-like constitutive properties indicates that for SOC73, a value of τ_v equal to about one tenth of its minimum critical damping value is sufficient. Therefore, we suggest

$$\tau_v = \frac{\Delta r}{10c}. \quad (77)$$

This equation may, at worst, lead to some oscillation near the energy source, a region in which we usually have little quantitative interest. Of course, further control over damping could be attained by allowing τ_v to be a function of position, stress, strain, etc.

To obtain a convenient final form for the threshold τ_v , recall that c is not necessarily a constant, but it is determined from k , G , and ρ by

$$c^2 = \frac{k(P) + \frac{4}{3}G}{\rho}. \quad (78)$$

To be conservative, we choose to use $c_{\min}$, the minimum value of sound speed with respect to variation in P . Furthermore, since Eq. (77) is developed for a shock width of five zones, we insert $W = 5\Delta r$ to give

$$\tau_v = \frac{W}{50 c_{\min}}. \quad (79)$$

In this way, the user can think in terms of the desired shock width. We obviously recommend that W be at least five zones for threshold damping. However, we can make W less if we want to, but the possibility of error increases. For variable zoning, W should also be about five zone widths for the region of interest.

VISCOUS PORE COLLAPSE

In porous geologic materials, our attempts to produce the observed waveform damping by using Eq. (74) have been unsuccessful because it appears that the damping is porosity dependent; i.e., damping is large at low pressures but diminishes rapidly as porosity is permanently removed by compression. SOC73 does not currently model this behavior, but a model has been developed²⁵ which has been applied with some success²⁶ using an experimental version of SOC73.

SHEAR AND TENSILE FAILURE DAMPING

Recall from the previous section on shear failure that for brittle failure, two failure surfaces, I_v and I_t , are defined. When failure first occurs at $I_{2d}^{1/2} = I_v$, the stress deviators are reset, or relaxed, such that $I_{2d}^{1/2} = I_t$. It was stated that such a relaxation, for reasons of stability,

could not be allowed to occur instantaneously. To regulate the rate of deviatoric stress relaxation is to create a rate-dependent shear stress-shear strain model. The equation used in SOC73 to calculate deviators during brittle failure relaxation is

$$\dot{s}_i^* = \dot{s}_i - \frac{s_i}{\tau_m} \left(1 - \frac{I_f^*}{I_{2d}^{1/2}} \right), \quad (80)$$

where s_i is the elastic or trial deviator value as obtained from Eq. (24), and τ_m is called the Maxwell relaxation time, because the plane viscoelastic equivalent of Eq. (80) is a spring in series with a dashpot or a Maxwell solid.²⁴ Note that this system is a high-pass filter for shear. Rapid increases in shear stress are allowed, but slow changes are damped, as shown in Fig. 26. The parameter I_f^* is an effective failure surface which lies somewhere between I_v and I_f . It appears in Eq. (80) because, even with the more

continuous relaxation produced by the Maxwell damping, the sudden change of rate caused by switching from I_v to I_f proves, on occasion, to cause unwanted oscillations. We therefore chose to insert an effective failure surface, I_f^* , which has a smooth transition between I_v and I_f . We would like the position of this surface to depend on the extent of failure. For our convenience, we already have a measure of the extent of failure, namely ϵ_f . Therefore, let

$$\begin{aligned} I_f^* &= I_v - \frac{\epsilon_f}{\epsilon_0} (I_v - I_f) & \epsilon_f < \epsilon_0 \\ I_f^* &= I_f & \epsilon_f \geq \epsilon_0 \end{aligned} \quad (81)$$

where ϵ_0 is a threshold value of failure strain provided by the code user. The value of ϵ_0 can be thought of as the failure strain required for failure initiation. That is, a certain amount of damage must be done to a material before it deforms as if failed. A microphysical model of this behavior could be one where microcracks grow and coalesce before macroscopic, violent failure can proceed. This can be associated with the finite time and strain required for dislocation motion or grain sliding to occur. Values anywhere from $\epsilon_0 = 0.01$ to $\epsilon_0 = 0.1$ have proved successful in calculations. Note that Eq. (80) reduces to Eq. (50) if τ_m approaches zero because $\tau_m = 0$ removes the rate dependence.

Thus far, the discussion has involved only brittle failure. For ductile failure, because there is only one failure surface, $I_v = I_f = I_f^*$, and there is no stress relaxation in the sense of moving from one surface to another. However, if Eq. (80) were applied directly, there would be a

Fig. 26. SOC73 model for rate-dependent shear failure. Dashed lines show loading paths leading to failure. The upper brittle path has a larger Maxwell relaxation time than the lower.

stress overshoot during ductile failure with a return to the failure surface which depended on τ_m . To avoid an overshoot in SOC73, the material undergoing ductile failure must always remain on the failure surface (Fig. 26). This is achieved by an adjustment of the Maxwell relaxation time. We simply allow τ_m to become smaller, but approach Δt continuously as the brittle-ductile transition is approached. If the input value of the Maxwell relaxation time is called τ_{mo} , then

$$\tau_m = \tau_{mo} \left(\frac{l_v - l_f}{l_v} \right) \quad \tau_m > \Delta t \quad (82)$$

$$\tau_m = \Delta t \quad \tau_m \leq \Delta t$$

At the brittle-ductile transition, τ_m approaches Δt and in the ductile regime, stress relaxation occurs in exactly one time step. Thus, we have prevented overshoot, and either Eqs. (80) or (50) may be used to calculate stress in ductile material.

We use the same type of Maxwell damping for tensile failure. The equation for principal stress relaxation becomes

$$\dot{\sigma}_i = \dot{\sigma}_i - \frac{\sigma_i}{\tau_m} \quad (83)$$

Note here also, that Eq. (83) reduces to Eq. (51) for $\tau_m \rightarrow 0$, as it should.

RATE DEPENDENT FAILURE STRAIN

The rate dependencies in shear and tensile failure introduced above require changes to the previous static formulation for the calculation of ϵ_f . We now need the equation for the rate of change of ϵ_f . For the cases of brittle and tensile failure

$$\dot{\epsilon}_f = \frac{1}{2 G \tau_m} \left(\frac{1}{2d} - l_f^* \right) \quad (84)$$

For ductile failure, Eq. (64) still applies. However, Eq. (64) can be written

$$\dot{\epsilon}_f = \frac{1}{2 G \Delta t} \left(\frac{1}{2d} - l_f^* \right) \quad (85)$$

where Δt is the calculational time step. If Eq. (82) for τ_m is used in (84), Eq. (85) results in the ductile regime, so there is never a need to use Eq. (85) to find the failure strain rate; Eq. (84) will always suffice.

CHOOSING THE MAXWELL RELAXATION TIME

All of SOC73's failure routines use τ_m , the Maxwell relaxation time, as defined above. If more than one failure is occurring, multiple relaxations are allowed to take place, each with the same τ_m . How should the user choose τ_{mo} ? To ensure continuous relaxation in the highly brittle region; i.e., where l_v and l_f are greatly different, we should have $\tau_{mo} \gg \Delta t$. The situation appears to be similar to the determination of τ_v for the Q calculation. If a great deal of slow relaxation occurs in nature we can compare that data with experimental data and find τ_{mo} . However, if this is not the case, we must at least ensure that τ_{mo} is high enough above a threshold value in the brittle region so that nonphysical oscillations are prevented. As a rough guideline, consider a typical calculational time step

$$\Delta t_0 = \frac{\overline{\Delta r}}{\frac{1}{2}(c + c_{\min})} \quad (86)$$

where $\overline{\Delta r}$ is the median zone size, c is the initial sound speed and $c_{\min}$ is the minimum sound speed as found from Eq.

(78). This value, Δt_0 , is probably near to the largest Δt that could occur at times when failure is important. (Larger Δt 's might occur at late times in some prob-

lems, but then purely elastic behavior probably dominates.) We therefore conservatively suggest that $\tau_{mo} = \Delta t_0$ be used as the threshold value.

Summary

SOC73 is an improved version of SOC. Both codes have been equally successful at predicting time of arrival and peak values in the field. SOC73, however, is considerably better at predicting wave shapes because it has essentially eliminated the nonphysical discontinuities that tend to complicate results. SOC73 is formulated so that both high-frequency damping and failure can be accounted for in terms of a relatively few parameters, and with clear physical equivalents. We have introduced the concept of failure-associated strain to SOC73,

which may lead to a simple technique for predicting shock-induced damage.

The most important solid media constitutive models lacking in SOC73 are those involving shear-volume interactions and rate-dependent pore collapse. These could be easily added to SOC73. Less easily added, but perhaps important in the long run, are multiphase models of solids (including water) and thermal effects. The "evolutionary" goal of SOC73 modeling has been achieved, but important areas remain for future work.

Acknowledgments

The author wishes to thank Fran Petersen for her coding efforts. Also, Bob Terhune, Ted Butkovitch, Joe

Hearst, and Don Larson provided test problems and valuable criticism of results.

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