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A COMPUTATIONAL STUDY OF SHOCK PROPAGATION IN INDIANA LIMESTONE

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Simple mixture rules are used to calculate input parameters for an analytic equation of state package (ANEOS) to model saturated limestone as a homogeneous material. This method is used to determine changes in material parameters as the volume fraction of water in the rock changes. Hugoniots determined from these calculations are compared with experimental and theoretical results for saturated limestone. Ground shock calculations are also performed to model a deeply buried explosion in saturated limestone containing various amounts of water.

1. INTRODUCTION

This work considers computer simulations of undergound explosions in saturated limestone (calcite) and the influence of variability of material property on response of the medium. Average material properties are determined as a function of pore water content. The saturated rock is modelled as a homogeneous mixture of water and calcite, and simple mixture rules are used to determine input parameters for an analytical equation of state (ANEOS[1]). Section 4 describes Hugoniots calculated with ANEOS and compared with available experimental data. In Section 5, ANEOS is used in a one-dimensional wavecode (CHARTD[11]) to simulate explosions in saturated limestones. Input values for ANEOS are chosen to represent initial conditions of saturated limestone containing different amounts of water. The effect of varying water content on the attenuation of quantities such as stress and particle velocity is considered.

2. MATERIAL MODEL

The ANEOS equation of state used in these calculations allows for a thermodynamically complete and consistent material description. Pressure and energy are written as sums of contributions from: (1) atomic and electronic interactions at $T = 0$, (2) thermal motion of atoms and ions, and (3) thermal motion, excitation, and ionization of electrons. The first term is the cold curve; the other terms are found from theoretical models not discussed here.

At high pressures, Thomas-Fermi theory is used to determine the cold pressure. Low pressure states are calculated from material properties at P_0, T_0. At intermediate states an interpolation formula is used to connect these two regimes; input parameters are determined from the atomic numbers and masses or from the experimental Hugoniot.

A first or second order polymorphic phase change can be modeled in ANEOS. Required parameters include the density (2nd order) or densities (1st order) and the pressure at which the transformation occurs, along with the first and second derivative of pressure at the completion of the phase transition.

3. MIXTURE PARAMETERS

The saturated limestone is assumed to contain pores which are completely water-filled. Changes in the various material parameters are correlated with changes in water content, and effective properties of the saturated material are calculated. The method used to calculate the effective properties is given elsewhere[2]; this basic method is extended to calculate additional parameters ($U_s - u_p$ slope, phase transition parameters, etc.) not considered in the original work.

In thermal equilibrium, the specific volume is:

$$V = \lambda_1 V_1 + \lambda_2 V_2, \tag{1}$$

where 1 and 2 refer to the rock and water, respectively, and the λ's are mass fractions (with $\lambda_1 + \lambda_2 = 1$).

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The thermodynamic parameters α, β and C_p (thermal expansion coefficient, isothermal compressibility, and heat capacity, respectively) for the homogeneous mixture of water and rock are given by:

$$\beta V = -(\frac{\partial V}{\partial P})_T = \lambda_1 \beta_1 V_1 + \lambda_2 \beta_2 V_2, \tag{2}$$

where similar equations define αV and C_p.

Most parameters of the mixture, e.g., density (ρ_0), sound speed (C_0), and Gruneisen ratio (Γ_0) are calculated using the method of Duvall, et. al.[2]; the values vary monotonically with water content. See the work of Brown[10] for details. Additional parameters are defined below.

3.1 $U_s - u_p$ slope (S_1):

Second-order tangency of the Hugoniot and release isentrope at ρ_0, T_0, allows this slope to be calculated:

$$S_1 = \frac{\rho_0}{4C_0^2}(\frac{\partial^2 P}{\partial \rho^2})_S|_{\rho_0, T_0} + \frac{1}{2}. \tag{3}$$

This second derivative can be written as

$$\frac{\partial^2 P}{\partial \rho^2} = -V^2 \frac{\partial (C^2)}{\partial V} = -V^2 (\frac{2V\Psi - V^2(\frac{\partial \Psi}{\partial V})}{\Psi^2}), \tag{4}$$

where:

$$\Psi = \beta V - T\alpha^2 V^2 / C_p. \tag{5}$$

The derivative of (βV) can be further expanded as:

$$\frac{\partial(\beta V)}{\partial V} = \lambda_1(\beta_1 + V_1\beta_1')(\frac{\beta_1 V_1}{\beta V}) + \lambda_2(\beta_2 + V_2\beta_2')(\frac{\beta_2 V_2}{\beta V}), \tag{6}$$

where the symbol ($'$) indicates a derivative with respect to the specific volume of each constituent. Similar expressions are obtained for derivatives of (αV) and (C_p).

Figure 1 shows variation of S_1 with volume fraction of water. S_1 increases sharply as small amounts of water are added to the matrix, reaches a maximum when the volume fraction of water is slightly less than 5%, and then begins to decrease at a slower rate. This unusual variation of S_1 with volume fraction of water can be understood as the ratio of the volume derivative of the compressibility (numerator) and the compressibility (denominator).

These parameters describe the behavior of the water-rock mixture at ρ_0, T_0, however additional parameters are needed to account for polymorphic phase changes.

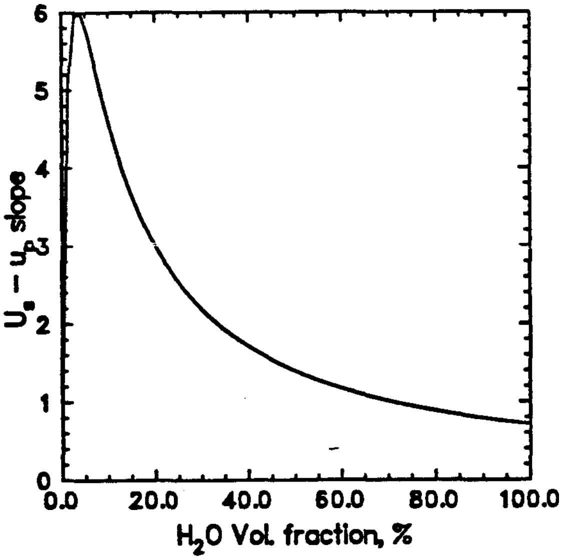

FIGURE 1

Variation of the $U_s - u_p$ slope of saturated limestone with change in the volume fraction of water.

ANEOS allows only one phase transition, but limestone has several phase changes in compression[4]. Transitions in the pressure range of about 1.5 to 1.8 GPa account for a large volume change; in dry calcite the total permanent volume change is about 10%. The decision was made to model a pseudo-transition which merges the total volume changes in this pressure range into a single transformation. This gives a Hugoniot curve which closely approximates the calcite II to calcite III transition, but the calcite III to aragonite transition is not modelled. Computed results show that this is not critical in modelling the compression of the saturated limestone.

3.2 Transition Densities ($(\rho_i)_{ctr}, (\rho_f)_{ctr}$):

Initial (i) and final (f) densities of the phase change are determined from an application of Equation 1:

$$(V_i)_{ctr} = \lambda_1 V_{i1} + \lambda_2 V_{i2}, \tag{7}$$

where V_1 is the specific volume of the rock matrix (calcite) and V_2 is a parameter which is approximately the specific volume of water at the transition pressure. V_2 is not the actual water volume because of a presumed hydrate reaction in which the mineral ikaite formed[4].

Parameters in (7) are determined from experimental data (quasi-static) of Heard, *et al.*[3], and from the Hugoniot of dry calcite. The final volume (V_f) of the transition can be determined from a similar equation. These two volumes increase monotonically with water content, eventually becoming equal. The phase change eventually looks like a second order, rather than first order transition.

3.3 Pressure Derivatives:

ANEOS requires input values of $(\frac{\partial P}{\partial \eta})$ and $(\frac{\partial^2 P}{\partial \eta^2})$ at the completion of the transition,where $\eta = \frac{\rho}{\rho_{00}}$ and $\rho_{00} = \rho(T = 0K)$. The first derivative is , within a factor of ρ_{00}, identical with the square of the sound speed and shows the same monotonic variation with water content. The second derivative can be written as:

$$\frac{\partial^2 P}{\partial \eta^2} = -\rho_{00}^2 \frac{\partial}{\partial \rho}(V^2 \frac{\partial P}{\partial V}) = (\frac{V}{V_{00}})^2 \frac{\partial (C^2)}{\partial V}, \qquad (8)$$

which is identical to Equation 4, within a factor of $-\rho_{00}^2$. Equations 4-6 can be applied to express the final result in terms of volume derivatives of the compressibility, heat capacity and thermal expansion coefficients of the individual constituents; however, these parameters must be evaluated at the temperature appropriate to the transition. The calculated second derivative varies with water content in a manner similar to the initial $U_s - u_p$ slope (Fig. 1).

Additional input parameters (Debye temperature, zero temperature separation energy and several critical point quantities) were kept at their default values. The melt energy was held fixed at the value for dry calcite. Yield strength of the saturated rock is important in determining material response; however, it depends on such things as pore pressure and chemical reactions. These effects are beyond the scope of this work. A yield strength of approximately 0.1 GPa was used in the ground shock calculations.

4. LIMESTONE HUGONIOTS

The above procedure was used to calculate the Hugoniots for four different initial densities of saturated limestone and compared with experimental data. Comparisons were also done with a theoretical description[4] of the limestone studied by Furnish[8].

In Figure 2, Hugoniots from calculations, experiments, and theory are in generally good agreement. However, agreement is poor with Furnish's data[8] at low pressures. This is apparently due to material strength effects, and must be considered in more detail.

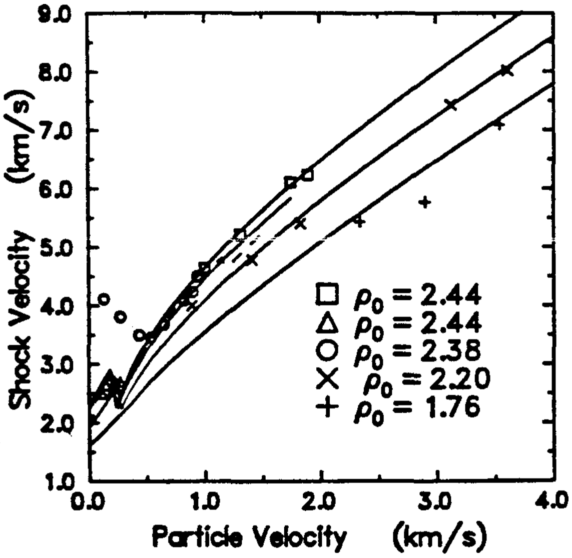

FIGURE 2

Hugoniots of saturated limestones: squares[7], triangles[9], circles[8], crosses[6], and saturated chalk: x's[5]. Solid lines are from ANEOS and dashed line is from theory[4] for $\rho = 2.38$.

5. GROUND SHOCK MODELLING

Spherically symmetric CHARTD calculations were done to model explosions ($\sim 2 \times 10^7 J$) in saturated limestone with initial water <u>volume fractions</u> (φ_2) of 10%, 15% and 20%.

Figure 4 shows peak radial stresses versus distance. Near the source, the model predicts small differences among the samples of different porosities. At lower pressures, there are noticeable differences among the curves: if the porosity is 15% ± 5%, then the distance at which the peak pressure decays to $0.1 GPa$ is uncertain by approximately ±50m.

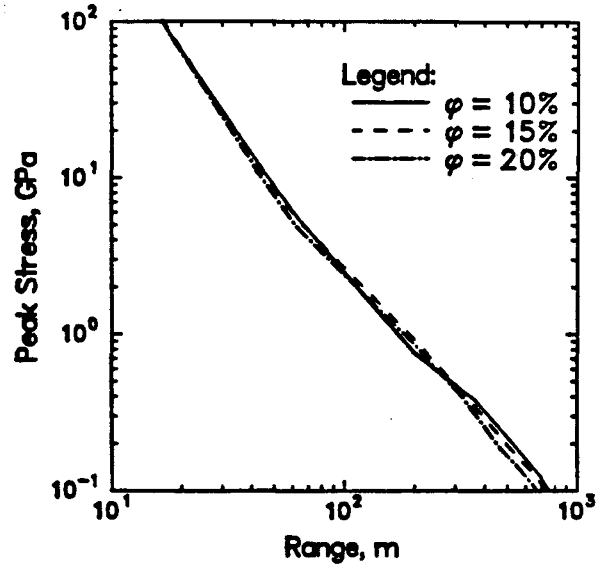

FIGURE 3

The decay of peak radial stress with propagation distance for saturated limestone with three different volume fractions of water.

Peak velocity curves (Figure 4) near the source are almost identical. At intermediate distances, there is significant separation among these curves. However, at $1km$ the three curves show negligible differences. From this result, measurements based on peak velocity, rather than peak stress, are relatively insensitive to these variations in volume fraction of water.

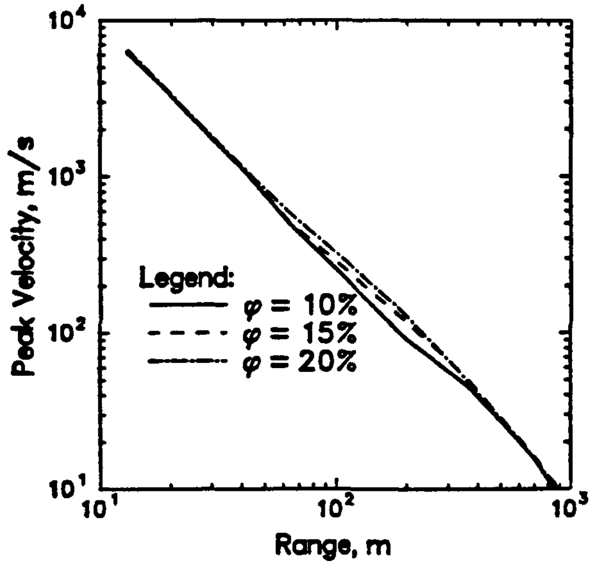

FIGURE 4
The decay of peak velocity with propagation distance for saturated limestone with three different volume fractions of water.

6. SUMMARY and CONCLUSIONS

ANEOS input parameters calculated with this simple mixture model give results which are in good agreement with available experimental and theoretical Hugoniots for a wide porosity range. However, agreement is poor for several low pressure data points; this needs to be explored further. Limestone experiences several phase transformations during shock compression, but the single phase change modelled by ANEOS gives good agreement with experimental data.

Peak stresses and velocities were calculated for spherically symmetric explosions in three different saturated limestones. Peak stress is apparently more sensitive to water content than is peak velocity.

There are several limitations to the method used in this study. Treating the saturated rock as a homogeneous, equilibrium mixture ignores the possibility of differences in fluid pressures and temperatures of the matrix and pore fluid. The presence of a pore fluid in a soil or rock can lead to pore pressures which have significant effects on material strength. Thermodynamic properties which depend o temperature can be considerably in error if a single temperature is used. This study only considered changes in the loading behavior (Hugoniots) due to water content. Release behavior is also important in determining the attenuation of peak values at the shock front. Experimental data show evidence of high pressure release shocks, apparently due to reverse phase changes which are not included in the ANEOS models.

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