Prediction of shock-induced cavitation in water

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Abstract. Fluid-structure interaction problems that require estimating the response of thin structures within fluids to shock loading have wide applicability. For example, these problems may include underwater explosions and the dynamic response of ships and submarines; and biological applications such as Traumatic Brain Injury (TBI) and wound ballistics. In all of these applications the process of cavitation, where small cavities with dissolved gases or vapor are formed as the local pressure drops below the vapor pressure due to shock hydrodynamics, can cause significant damage to the surrounding thin structures or membranes if these bubbles collapse, generating additional shock loading. Hence, a two-phase equation of state (EOS) with three distinct regions of compression, expansion, and tension was developed to model shock-induced cavitation. This EOS was evaluated by comparing data from pressure and temperature shock Hugoniot measurements for water up to 400 kbar, and data from ultrasonic pressure measurements in tension to -0.3 kbar, to simulated responses from CTH, an Eulerian, finite volume shock code. The new EOS model showed significant improvement over pre-existing CTH models such as the SESAME EOS for capturing cavitation.

1. Introduction
The Tillotson Equation of State (TEOS) was originally defined by Tillotson [1] to better predict shock pressures in metals [2] during hypervelocity impact. For this class of problems, materials can change phase upon compression, such as transitioning to a different solid polymorph or melt, and change phase upon release by melting or vaporizing. The TEOS was formulated to treat hypervelocity impacts with sufficient shock energy to cause vaporization upon release. Since the development of the original model in the early 1960’s, which included separate regions for compression and expansion, a number of modifications have been made to the analytical model to treat solid-solid polymorphs and geological materials, and to provide improvements to the gas-solid mixing region, for example.

Whereas these improvements have been for solid materials, the author has also contributed significant improvements to the expansion region of the TEOS by introducing additional regions in the density-energy phase space that closed previously unpublished gaps, as given by Brundage [3]. With this additional coverage of the phase space, the analytical model was augmented with a cavitation model to treat the two-phase behavior of liquids expanded to the vapor pressure. It has been known for over a century that liquids such as water can sustain large negative pressures in metastable thermodynamic states before cavitation occurs [4]. Hence, this paper introduces a third independent region in the density-energy phase space to capture tensile behavior, and the revised model is evaluated by comparing the computational results to experimental data for water.
2. Rankine-Hugoniot Jump Conditions for the TEOS

Shock Hugoniot data compiled in plane wave experiments, such as free surface velocity and shock velocity, are used to calculate thermodynamic parameters behind the shock front for single shocks by applying the Rankine-Hugoniot (RH) jump conditions [5]. These data, which represent the locus of end states, assuming thermodynamic equilibrium, are used to fit a RH curve defined from the EOS surface.

The TEOS equilibrium surface in compression is defined as

\[ p(\rho, E) = \left[ a + \frac{b}{(E/E_0\eta^2 + 1)} \right] \rho E + A\mu + B\mu^2 \quad (\rho \geq \rho_0, E \geq 0) \quad (1) \]

with \( \eta = \rho/\rho_0 \) and \( \mu = \eta - 1 \), where the constants \( a, b, E_0, A, B \) are adjusted to provide the best fit to shock Hugoniot data. The RH jump condition derived from the conservation of energy is defined as

\[ E_H(\rho) = \frac{1}{2} P_H(\rho) \left[ \frac{1}{\rho_0} - \frac{1}{\rho} \right] \quad (2) \]

where the \( E_H \) and \( P_H \) represent the thermodynamic variables behind the shock. Since these end states are assumed to be in equilibrium, the \( P_H-\rho \) relation, or Hugoniot curve can be defined by equating \( E \) with \( E_H \) and \( P \) with \( P_H \) in equations (1) and (2), respectively, given the initial state. Accordingly, by substituting equation (2) into (1) and solving algebraically for \( P_H \) yields the following expression:

\[ P_H(\rho) = -\frac{b_H + (b_H^2 - 4a_H c_H)^{1/2}}{2a_H} \quad (3) \]

where the coefficients \( a_H, b_H, \) and \( c_H \) are defined as

\[ a_H(\rho) = \frac{S - a\rho S^2}{k} \quad b_H(\rho) = (1 + b)k - \frac{S}{k} \quad c_H(\rho) = l \quad (4) \]

and the variables \( S, k, \) and \( l \) are given by

\[ S(\rho) = \frac{1}{2} \left( \frac{1}{\rho_0} - \frac{1}{\rho} \right) \quad k(\rho) = E_0\eta^2 \quad l(\rho) = A\mu + B\mu^2 \quad (5) \]

For temperatures below an electron-volt (11,604 K), the internal energy of a simple compressible substance, assuming constant specific heat, can be defined as

\[ E(\rho, T) = E_C(\rho) + C_V(T - T_0) = E_H(\rho) + C_V(T - T_H) \quad (6) \]

The cold energy, \( E_C \), which represents the equilibrium state of a solid at zero temperature, can be calculated from the thermodynamic definition of pressure

\[ \frac{dE_C}{d\rho} = \frac{P(\rho, E_C)}{\rho^2} \quad (at \ \rho = \rho_0, \ E_C = 0) \quad (7) \]

Eliminating \( E \) (or \( T \)) in equation (6) yields the following expression for \( T_H \):

\[ T_H(\rho) = T_0 + \frac{E_H(\rho) - E_C(\rho)}{C_V} \quad (\rho \geq \rho_0) \quad (8) \]
Now that relationships for the Hugoniot pressure and temperature have been defined, values of the coefficients $a$, $b$, $E_0$, $A$, $B$ can be obtained using available thermodynamic and shock Hugoniot data. The parameters for water are included in table 1.

**Table 1.** Tillotson Equation of State Parameters for Water in Compression.

| $\rho_0$ (g/cm$^3$) | $a$ | $b$ | $A$ (kbar) | $B$ (kbar) | $E_0$ ($10^{12}$ erg/g) |
|---------------------|-----|-----|------------|------------|-------------------------|
| 0.998               | 0.7 | 0.15| 21.8       | 132.5      | 0.07                    |

### 3. Results and Conclusions

Measurements of the pressure and temperature shock end states for water [6, 7] are compared with the RH relationships previously given and the responses from CTH [8] using various equations of state, i.e. the Tillotson, Mie-Gruneisen, and SESAME models, for a symmetric impact simulation. As shown in figure 1, all of the simulated results are within the scatter of the data up to 400 kbar; however, the best comparison to the pressure data is given by the Tillotson EOS. At least up to the extent of the data, the SESAME EOS, which has a variable specific heat, provides the best fit to the temperature data. This is not unexpected, given that temperatures, especially for liquids, are sensitive to the specific heat; hence, suggesting the addition of variable specific heat to the Tillotson EOS to better represent shock temperatures in future model revisions.

![Figure 1](image1.png)

**Figure 1.** Comparison of shock (a) pressure and (b) temperature data to Hugoniot relationships and simulations from CTH using various equations of state.

To capture the effects of shock-induced cavitation in fluids, where the interaction of reflected waves can cause the fluid to stretch and rupture in response to tensile forces, a tensile region was added to the Tillotson EOS. According to Davitt [9], who conducted ultrasonic sound speed measurements in water, the fluid was allowed to stretch in a metastable state to a pressure of -0.3 kbar at a temperature of 296 K before rupturing by releasing vapor and dissolved gases. Hence, the modeling approach for allowing the fluid to experience negative pressures before cavitation is consistent with the experimental evidence.

To demonstrate this new approach, a computational spall experiment was setup using a one-dimensional CTH calculation where a 2-cm thick flyer (water) at 400 cm/s impacted a 4-cm thick target (water). At the spall plane, once the pressure drops below the cavitation threshold pressure, instead of inserting void, vapor is inserted at the vapor pressure of water, a user-defined parameter set here to 0.05 bar. The results of this simulation are given in figure 2.
Figure 2. Axial pressure distribution for computational spall example using Tillotson EOS with cavitation (a) at the impact plane, (b) at the spall plane, (c) at the spall plane using SESAME 7150.

In figure 2(a), the pressure wave profiles at impact are shown, recovering the calculated impact pressure of 29.6 bar. At a later time of 44 µs, after spall leading to cavitation at the spall plane (the target mid-plane) has occurred, the peak pressure is 0.05 bar, as shown in figure 2(b). This impact scenario was also evaluated using SESAME 7150, the tabular EOS for water in CTH. Here, a slightly higher impact pressure of 31.5 bar was predicted, and the vapor pressure was not recovered across the spall plane, as shown in figure 2(c). Other SESAME equations of state were evaluated, both with and without tensile regions, but none of them reproduced both the calculated impact pressure and the vapor pressure across the spall plane at the time of fluid rupture. Although those results are not reported here, a specific model for cavitation is needed to capture this phenomenon in hydrocode simulations, with the level of sophistication dependent upon the application.

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