Modelling the equation of state of a graded density impactor

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Abstract. There is a requirement for off-Hugoniot data to validate material and equation of state models. One technique is to use projectiles with graded shock impedance layers in a gas gun to impact a target and apply a ramp loading. To accurately design a pressure profile to be applied to the target the impactor must be accurately characterised and modelled. Modelling also provides an assessment of whether lateral rarefactions will hinder the experiment, and increases confidence in the analysis of the results obtained. This paper considers several methods for calculating the equation of state of layered mixtures for application to the modelling of graded density impactors.

1. Introduction
There is a requirement for off-Hugoniot data to validate material models. Barker [1] developed a technique using projectiles with graded shock impedance layers in a gas gun to apply a ramp loading to the target. More recently researchers at LLNL [2,3] have developed techniques for manufacturing graded density impactors (GDIs) that consist of thin layers of the order of a few tens of microns thick. The aim of this paper is to consider how these GDIs may be modelled in hydro-codes since this is an important requirement in designing experiments.

2. Methods for Calculating the Mixture Hugoniot
The equation of state (EoS) for each component of the mixture is taken from Steinberg [4]. The Steinberg EoS models assume a linear relationship between the shock velocity, $U_s$, and particle velocity, $U_p$, as shown in equation (1), where $C_0$ is the room temperature and pressure (RTP) sound speed and $s$ is the slope of the Hugoniot.

$$ U_s = C_0 + sU_p $$

Three options for calculating the mixture Hugoniot are considered below. It is assumed in all cases that the layered mixtures are not chemically bonded. In the notation used throughout this paper the subscript $m$ and $i$ refer to the mixture and components of the mixture respectively.

2.1. Option A: Pressure-Temperature Equilibrium
By assuming that the mixture is in pressure, $P$, and temperature, $T$, equilibrium the EoS is calculated by equating the specific volume, $v$, and internal energy, $E$, of the mixture to be the mass weighted, $\alpha$, sums of the specific volumes and internal energies of the individual components, as shown in equations (2) and (3).
\[ v_m(P, T) = \sum \alpha_i v_i(P, T) \]  
\[ E_m(P, T) = \sum \alpha_i E_i(P, T) \]

### 2.2. Option B: Additive Volume Method

For this method, it is assumed that each component of the mixture lies on its own Hugoniot and the volume of the mixture Hugoniot, \( v_{\text{H}} \), at a given pressure is obtained as a mass weighted sum of the volumes of the components at the same pressure. Thus no account is made for the temperature of the components on their Hugoniots.

\[ v_{\text{H}}(P) = \sum \alpha_i v_{i\text{H}}(P) \]

### 2.3. Option C: Determine parameters for the mixture EoS

The mixture EoS form used is the same as the component EoS, but two methods are considered for obtaining the parameters for the \( U_s-U_p \) relation. However, in both methods the specific volume of the mixture is given by

\[ v_m = \sum \alpha_i v_i \]

the energy by

\[ E_m = \sum \alpha_i E_i \]

and for the Gruneisen parameter, \( \Gamma \), of the mixture equation (7) is assumed

\[ \Gamma_m = \Gamma_{0m} - a_m \epsilon \]

where \( \Gamma_0 \) and \( a \) are constants and \( \epsilon \) is the volumetric strain. Differentiating equation (6) with respect to pressure, and using \( \frac{\partial E}{\partial P} = \frac{\nu}{\Gamma} \) gives equation (8), which is used to obtain \( \Gamma_{0m} \).

\[ \frac{v_m}{\Gamma_m} = \sum \frac{\alpha_i v_i}{\Gamma_i} \]

The parameter \( a_m \) in equation (7) may be obtained by fitting to \( \Gamma_m \) evaluated at large densities. However, it was found that this result was very close to that obtained using equation (9).

\[ a_m = \sum \alpha_i a_i \]

#### 2.3.1. Option C: AWE method for determining \( U_s-U_p \) relation

By assuming pressure equilibrium the sound speed of the mixture is calculated using equation (10).

\[ \frac{1}{(\rho_{0m}c_{0m})^2} = \sum \frac{\alpha_i}{(\rho_{0m}c_{0i})^2} \]

The strain of the mixture is calculated using equation (11) and the pressure on the Hugoniot using equation (12), where \( v_0 \) is the specific volume at RTP.

\[ v_{0m}e_m(P) = \sum \alpha_i v_0 e_i(P) \]
\[ P = \frac{C^2_0 \varepsilon}{v_0 (1 - s \varepsilon)^2} \]  

Differentiating equations (11) and (12) to obtain expressions for \(\frac{d^2 \varepsilon}{dP^2}\), and equating terms at \(P=0\) and \(\varepsilon=0\), produces equation (13). This is used to obtain \(s_m\).

\[ \frac{V_{0m}^2 s_m}{C^2_{0m}} = \sum \frac{\alpha_i V_{0i}^2 s_i}{C^2_{0i}} \]  

The same methodology may also be used to obtain expressions for EoS parameters using the Steinberg cubic \(U_r-U_p\) form [4].

### 2.3.2. Option C: Batsanov’s method for determining \(U_r-U_p\) relation

Batsanov [5] calculates \(C_{0m}\) and \(s\) using equations (14) and (15) respectively, where \(\beta_0\) is the volume fraction at RTP.

\[ \frac{1}{C_{0m}} = \sum \frac{\beta_0}{C_{0i}} \]  

\[ \frac{1}{s_m} = \sum \frac{\beta_0}{s_i} \]  

### 3. Mixture EoS Comparisons

Four metallic mixtures of varying composition were calculated using the methods discussed above; these were Ta-Nb, Nb-V, V-Ti, and W-Mg. These mixtures were chosen because they were used in a GDI test case, the details of which are provided in section 4.

The AWE method produces lower values for \(C_{0m}\) and higher values for \(s_m\) than the Batsanov method. For Ta-Nb and Nb-V mixtures, these differences are small but for W-Mg mixtures these differences are large; this is shown in figures 1 and 2.

**Figure 1.** Sound speeds calculated by mixture formulae for W-Mg.

**Figure 2.** Hugoniot slope calculated by mixture formulae for W-Mg.

Figures 3 and 4 show calculated Hugoniots for 50/50 weight percentage compositions of Ta-Nb and V-Ti respectively. The pressure-temperature equilibrium and additive volume methods show good agreement; despite large differences in temperature the differences in volume between the two methods are small. Although these methods also show good agreement with the AWE and Batsanov calculations for the Ta-Nb composition, poor agreement is observed for the V-Ti mixture, which does
not show a linear $U_s-U_p$ relation. This is a consequence of the non-linear $U_s-U_p$ relation assumed for the Ti EoS because of a low pressure solid-solid phase transition. Increasing the AWE method to a cubic $U_s-U_p$ form does not improve this comparison.

Figures 3 and 6 show calculated Hugoniots for two W-Mg mixtures. The Batsanov method shows poor agreement with the alternative methods for the initial $C_{0m}$. For the 90/10 weight percent mixture, the pressure-temperature equilibrium is non-linear and thus the AWE method needs to be extended to the cubic form to show good agreement.

4. Application to Hydro-code Test Case
The methods for calculating a mixture were applied to a hydro-code test case featuring a GDI. This test case is designed to apply an initial shock followed by a ramp loading to a tantalum target. The thickness of the tantalum target, the GDI, and the tantalum backing plate of the impactor are 2.5 mm, 4.1508 mm, and 1 mm respectively. The GDI consists of 62 layers and contains mixtures of W-Mg, V-Ti, Nb-V, and Ta-Nb. The first layer of pure magnesium is 1.0508 mm thick but all additional layers are of the same thickness (0.0508 mm). The impact velocity is 0.4 cm/µs. Strength was modelled [4] for the pure magnesium and pure tantalum cells only.

The pressure at the impactor-target interface for the hydro-code calculation is shown in figure 7. The Batsanov method has a steeper rise due to the large sound speeds calculated for the W-Mg mixtures using this method. At approximately 0.5-0.6 µs an anomalous feature is seen in the pressure profile. The cause of this feature was traced back to the change in the composition of the GDI layers from a W-Mg to a V-Ti mixture. Figure 8 shows the acoustic impedance, $Z$, for the layers of the GDI, and at this change in composition a steep change is calculated in the acoustic impedance. However, if the impedance was calculated using equation (16) then no large change in impedance is observed, as
shown in figure 8. The concern is that an anomalous feature in a GDI experiment could be falsely attributed to physical measurement, i.e. evidence of a phase transition. Thus accurate models of GDIs are needed to increase confidence in the analysis of these experiments.

\[ Z_m = \sum \beta_i Z_i \]  

(16)

5. Conclusions
This note has described several methods for modelling the EoS of a GDI. However, an implicit assumption that the EoS of the components of the mixture are accurate has been made. In particular, the representation of the isentrope of these models should be investigated.

The pressure-temperature equilibrium and additive volume methods produced similar results. This has been explained by an insensitivity of the mixture volume to the component temperatures.

Of the two methods considered for determining parameters for a mixture EoS, the AWE method is recommended in preference to the Batsanov method. This is because the AWE method showed good agreement with the pressure-temperature equilibrium method, with the exception of vanadium-titanium mixtures. This was due to the non-linear \( U_S-U_P \) relation for the titanium EoS. Because of the complexity in modelling GDIs, it is recommended that materials with low pressure phase transitions are avoided during the manufacturing of a GDI.

The effects of strength in the mixed layers have been ignored in this note. In the first instance a simple mixture treatment could be applied. This would be easier to incorporate with the AWE method than the pressure-temperature equilibrium method. It is also probable that GDI layers will have a degree of porosity that must be taken into account. All these problems indicate that experiments are essential to validate the modelling of both the individual mixture layers and the whole GDI.

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