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Abstract

The Hugoniot data on fused silica that are displayed on page 321 of the well-known volume “LASL Shock Hugoniot Data, Stanley P. Marsh, Editor” are fit to the EOS form 2 such as is used in CALE and other hydrocodes. Two fits are given: one to represent that data set over its full range (up to 84 GPa (840 kbar)) as well as a better fit for the pressure range below about 33 GPa (330 kbar). These EOSs have the strong point of being relatively simple for the user to implement and should be used to roughly represent the beyond-elastic response of fused silica in hydrocode simulations. They will not correctly reproduce the complex multiple-wave ramp-shock structure known to exist in fused silica at lower pressures.

Method and Results

The scope of this work is to report fits of the Hugoniot data for fused silica as displayed on pages 321 to 323 of reference 1 to an EOS form 2 (seven-term polynomial) equation of state [2] such as is used in the CALE hydrocode. Fused silica is a material with unusual properties and the fused silica Hugoniot data displayed in reference 1 deviate strongly from that of a typical material. It is difficult to fit this data set with a single fit. Two fits are reported: A fit over the full range of the data (up to 84 GPa) but best suited for the range between 33 and 84 GPa, as well as a fit which is better suited to pressures below 33 GPa. Frequently the EOS form 4 (Gruneisen EOS) is a more convenient representation of Hugoniot data. We also attempted a form 4 fit [3] but the form 2 appeared in this special case of fused silica to fit substantially better and hence was used here.

The EOS form 2 format is:

$$P = A_0 + A_1\mu + A_2\mu^2 + A_3\mu^3 + (B_0 + B_1\mu + B_2\mu^2)E$$

The independent variable μ is defined to be $(\rho/\rho_0 - 1)$ where ρ is density and ρ_0 is the reference density. According to the usage of reference 2 the independent variable E above is not the specific energy in the usual sense (i.e. energy per unit mass) but is instead “energy per reference volume”, which is equivalent to ρ_0 *(specific energy). P , A_0 , A_1 , A_2 , A_3 , and E as defined above have the units Mbar, whereas μ , B_0 , B_1 , and B_2 are dimensionless.

The variables μ and E are not independent along the shock adiabat (i.e. the Hugoniot) but are interrelated through the Rankin-Hugoniot relation [4,5]:

$$E_H = \frac{1}{2} P_H \mu_H / (\mu_H + 1)$$

This is a statement of energy conservation during the shock compression process and the subscript “H” signifies that the above interrelationship between E , P , and μ holds only along the shock adiabat. In the case of Hugoniot data this allows the elimination of E so that Hugoniot data can be fit knowing P_H only as a function of μ_H [6].

For the principal Hugoniots of solids or liquids the parameter A_0 is one atmosphere, which for all intents and purposes is equivalent to zero and we force A_0 zero in the fit. We did not use the parameter B_2 , setting it to zero. The parameter B_0 is the value of Gruneisen gamma for the reference, or uncompressed state. With B_2 set to zero B_1 becomes the limiting value of Gruneisen gamma at infinite μ . Setting the parameter B_1 equal to zero is equivalent to the commonly made constant (gamma / volume) assumption. This assumption gives a limiting value (as μ goes to infinity) of gamma which goes to zero, which is too small. Setting $B_1 = B_0$ is equivalent to the constant gamma assumption. This will give a limiting value of gamma which is usually too large (but as we shall see in the special case of fused silica, too small), since gamma for typical materials starts out around 1.5 to 2, whereas there is experimental and theoretical support that the limiting value of gamma should be around 0.5 to 2/3 [7].

B_0 is readily computed based on common thermodynamic data [8]:

$$B_0 = \frac{\alpha B_S}{\rho C_P}$$

B_S is the isentropic bulk modulus, α is the volume expansivity, ρ is (initial) density, and C_P is the specific heat at constant pressure. For isotropic solids such as fused silica B_S/ρ is readily computed from the longitudinal and shear sound speeds [9]:

$$\frac{B_S}{\rho} = C_L^2 - \frac{4}{3} C_S^2$$

So that:

$$B_0 = \alpha \left(C_L^2 - \frac{4}{3} C_S^2 \right) / C_P$$

The longitudinal and shear sound speed are taken from what was quoted in reference 1 to be 5960 and 3770 m/s, respectively. The constant-pressure specific heat is taken as 730 J/kg/°K, based on the average of several values from the literature. The linear thermal expansivity is 0.55 E-6/°K based on the average of several values from the literature. This would give 1.66 E-6/°K for the volume thermal expansivity. Thus B_0 evaluates to 0.0377,

an extremely low value relative to typical materials. This is due to the atypically low value for the thermal expansivity (in fact it is one of the properties for which fused silica is well known). We decided to assign B_I the value 0.667 as it would give a gamma at large μ closer to the correct limiting result expected by theory.

Fitting Procedure

The Hugoniot data is readily converted into P, μ space using the mass and momentum conservation relationships for 1-D steady waves [6]:

$$\rho(U_S - u_p) = \rho_0 U_S \quad \text{mass conservation}$$

$$P = \rho_0 U_S u_p \quad \text{momentum conservation}$$

(U_S is shock speed, u_p is particle speed, pressure ahead of the shock front is zero, and the material ahead of the shock front is at rest) together with the definition of μ . Thus we have the Hugoniot data plotted as P_H versus μ . We set $B_0 = 0.0377$ based on fused silica thermodynamic data and $B_I = 0.667$ based on theoretical guidance and experimental evidence from other materials as described above. Hence B_0 and B_I are treated as fixed constants during the fitting routine. We form the function $f(\mu)$ from the Hugoniot pressure $P_H(\mu)$ as follows:

$$f(\mu) = P_H(\mu) \left[1 - \frac{1}{2} (B_0 + B_I \mu) \frac{\mu}{\mu + 1} \right]$$

and we map the data from P_H to f versus μ according to the above.

Figure 1 shows the LASL data plotted as both f and P_H versus μ .

Then fit the data to the fit function:

$$f(\mu) = A_0 + A_1\mu + A_2\mu^2 + A_3\mu^3$$

A_1 , A_2 , and A_3 being fit parameters and also the desired coefficients of EOS form 2. This fit was done using the curve fitting routine in the plotting software IGOR PRO (WaveMetrics, Inc., Lake Oswego, OR) for two different μ ranges. Figure 2 shows the fit in f, μ space for the full LASL data range.

Figure 3 shows the same fit of Fig. 2 mapped back into the U_s, u_p range in which Hugoniot data are commonly reported.

The coefficients for the full data range fit (to 84 GPa) are:

A_0	0.	held fixed
A_1	0.8737	+/- 0.128
A_2	-1.7087	+/- 0.307
A_3	1.1857	+/- 0.18
B_0	0.0377	held fixed
B_1	0.667	held fixed
B_2	0.	held fixed

If the fused silica EOS is used in a simulation in which the maximum pressure in the fused silica component is not expected to significantly exceed 33 GPa (330 kbar), then a better fit to the data over a reduced μ range (0. to 1.) can be obtained. This fit is:

A_0	0.	held fixed
A_1	0.61966	+/- 0.012
A_2	-0.7551	+/- 0.0363
A_3	0.42164	+/- 0.0262
B_0	0.0377	held fixed
B_1	0.667	held fixed
B_2	0.	held fixed

Figures 4 and 5 display this latter fit overlaid with the data in f, μ and U_s, u_p space, respectively.

Figure 4: lower range fit (to 33 GPa (330 kbar))

Figure 5: lower range fit mapped back to $U_s - u_p$ space.

It is instructive to plot both the data and fits in $p - v$ space, and this is displayed in Figs. 6 and 7. The low range fit has a very slight upward convexity anomaly that persists to at least 17 GPa. It is not obvious in Figs 7 and 8 but shows up in simulations as a tendency for a compression wave at low pressures to gradually evolve into a ramp. On the other hand the upward convexity anomaly is very obvious in the full range fit and as a result the ramp distortion will be more pronounced. We show in Appendix A that to the extent that the loading curve approximates the principal isentrope the region of the convexity anomaly will result in the formation of a ramp wave in compression and shock wave in rarefaction.

Figure 6: $p-v$ plot of the data and the two EOS fits, to 0.46 Mbar

Figure 7: p - v plot of data and the two EOS fits over full range of data.

1-D simulations using the proposed fits.

Although no extensive testing was performed, four CALE simulations of 1-D symmetric impact were done just to give a feel for the wave profiles which will result from the proposed EOSs. A 0.5 cm thick impactor was impacted on a 2.5 cm thick sample using the same material for both impactor and sample. Two different impact velocities were used: 0.3 cm/ μ s and 0.5 cm/ μ s. Lagrange gauges (*i.e.* gauges that move with the flow) of particle velocity were imbedded at 0.5, 1.0, and 1.5 cm into the sample, relative to the impact plane as shown in Fig. 8. Simulations at 6 zones/mm and 10 zones/mm were compared and demonstrated convergence. The 10 zone/mm results are shown in the following figures.

Fig 8: cartoon of the 1-D impact simulation test.

Figure 9 show an impact to 17 GPa (0.3 cm/μs impact speed) in the low range fit material. There is a gradual but distinct compression ramp development and a clear rarefaction shock, both extending up to the full 17 GPa load. Figure 10 loads the low range fit impact loaded to 30 GPa. By this pressure, the compression ramp is fully overdriven by a normal shock wave but the anomalous nature of the fit still manifests itself in the still-present rarefaction shock as the material unloads below 19 GPa.

Figure 9: Wave profiles from low range fit under impact loading to 17 GPa.

Figure 10: Wave profiles from low range fit under impact loading to 30 GPa.

Figure 11 displays the full range fit loaded to 30 GPa. This pressure is not quite sufficient to completely overdrive the compression ramp of this fit, and this is not surprising given the (rather too high) speed of 6.3 km/s for the foot of the wave as can be seen in Fig. 3. Similar to the low range fit the rarefaction fan develops into a rarefaction shock as the pressure drops below 18 GPa.

Figure 11: Wave profiles from full range fit under impact loading to 30 GPa.

Suggestions regarding the use of these fits.

You may have heard that fused silica displays ramp compression wave behavior and it would be tempting to conclude that the ramp wave behavior demonstrated by these fits is an accurate representation of real ramp wave behavior in fused silica, but that is not so. Fused silica is in fact known for ramp wave behavior but it is in the intense and persistent elastic precursor that this behavior is seen. This precursor gives a ramp compression wave up to 3.8 GPa when shocked [10,11]. These fits presented here will not mimic the detailed ramp-wave elastic-plastic wave structure in fused silica. The reader is referred to Wackerle [10] and Barker and Hollenbach [11] for these details and an appropriate stress – strain relationship to model the precursor.

These EOS fits will roughly get the final pressure and density correct in hydrocode simulations. They will not at all correctly capture the true multi-wave ramp – shock structure known to exist in fused silica. References 10 and 11 are excellent sources for the details of the true wave structure. Wave arrival times should be reasonably accurate for the full range data above 34 GPa but only approximate for other cases.

Wackerle presented what he calls “strong evidence” for fused silica suffering a total loss of strength and rigidity beyond its elastic limit, becoming fluid-like. Consider setting strength to zero in the fused silica.

Appendix A: The principal isentrope in p - v space and ramp compression / shock rarefaction waves.

Rayleigh had known that the isentrope of a fluid had to have the form:

$$\frac{dp}{d\rho} = \frac{A}{\rho^2}$$

(“ A ” being a constant) for a pressure wave of finite amplitude to travel without distortion within that fluid [12] and in fact he attributed this result to earlier work by Earnshaw [13]. In p - v space the above statement is equivalent to:

$$\frac{dp}{dv} = -A$$

(same “ A ”) and therefore:

$$\frac{d^2 p}{dv^2} = 0$$

is the condition for distortionless propagation in p - v space. For typical materials the second derivative of p on v is greater than zero (i.e. the curve of p versus v is “concave up”), leading to the usual compression shock and rarefaction fan behavior. The “upward convexity anomaly” is mathematically:

$$\frac{d^2 p}{dv^2} < 0$$

The method of characteristics is the most straightforward path to demonstrate that the convex-up anomaly in the isentrope leads to compression ramps and rarefaction shocks. Considering a simple forward-facing wave one shows that the C+ characteristics (the trajectories in a - t space for a given pressure or amplitude level of the forward-facing wave) converge or cross for a rarefaction and diverge for a compression wave.

From the discussion of plane isentropic flow in Zel'dovich and Razier the differential equation for the C+ characteristics in Lagrange coordinates is [14, 15]:

$$\frac{da}{dt} = \frac{\rho}{\rho_0} c$$

Where “ a ” is the Lagrange coordinate. For “ c ,” the speed of sound, we can substitute:

$$c = \sqrt{\frac{dp}{d\rho}} = v \sqrt{-\frac{dp}{dv}}$$

so that:

$$\frac{da}{dt} = \frac{1}{\rho_0} \sqrt{-\frac{dp}{dv}}$$

For the forward-facing simple wave it can be shown [16] that the C+ characteristics are all straight lines but they don't necessarily all have the same slope. When dp/dv is constant, the C+ characteristics are all parallel (they then do all have the same slope, the same value of da/dt , independent of specific volume “ v ”) and compression and rarefaction waves of arbitrary amplitude propagate without distortion as was deduced by Earnshaw and Rayleigh. In a compression wave “ v ” decreases with increasing time. Under the anomaly condition this implies dp/dv becomes less negative, meaning da/dt becomes smaller in the next increment of time. If da/dt becomes smaller with increasing t then the characteristics are diverging and a compression wave will fan-out. On the other hand a rarefaction means “ v ” increases with time and the exact same line of reasoning shows the characteristics will eventually intersect leading to the formation of a rarefaction shock [Fig. 12].

Figure 12: The C+ characteristics in a - t space. Case 1: The v_1 and v_2 characteristics intersect. A shock wave will nucleate between states v_1 and v_2 . Case 2: The v_1 and v_2 characteristics run parallel. The wave between v_1 and v_2 will propagate without distortion. Case 3: The characteristics diverge and the wave will fan-out between v_1 and v_2 . Here v_1 and v_2 are two different specific volumes (or two different amplitude levels of the wave.)

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- 4 "Shock Wave Compression of Condensed Matter: A Primer", J.W. Forbes, report UCRL-MI-203449, 2004, p. 5, 151
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approximates the isentrope well enough to not make this distinction and we use the above energy conservation relationship without regard to the ramp or shock nature of the wave. The same justification applies to the (slight mis)use of the steady mass and momentum conservation equations. Ramp waves are not steady and this usage is therefore only approximate under those conditions.

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- 14 “Physics of Shock Waves and High-Temperature Hydrodynamic Phenomena” Ya. B. Zel’dovich and Yu. P. Razier (Academic Press, San Diego, 1966) p. 19
- 15 The Lagrange coordinate “a” has units of length and is used to index a particular mass element in a problem. “a” is in fact the initial position “ x_0 ” of the mass element it refers to.
- 16 p. 28 of reference 14