APPROXIMATIONS TO THE HUGONIOT P-V CURVE OF FUSED QUARTZ

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1. The Hugoniot U_S, U_P relation has the form

$$U_S = a + bu + cu^2 + du^3 \tag{1}$$

Then

$$P = \rho_o au + \rho_o bu^2 + \rho_o cu^3 + \rho_o du^4 \tag{2}$$

A direct relation between P and V is desired. There are various measures of V in common use; two are

$$\eta = 1 - V/V_o \tag{3}$$

$$x = (V_o/V) - 1 \tag{4}$$

A form frequently used is

$$P = \alpha x + \beta x^2 + \gamma x^3 + \delta x^4 \tag{5}$$

The jump condition for mass conservation can be written as

$$\frac{U_S}{U} = \frac{1}{\eta} = \frac{x+1}{x} \tag{6}$$

The coefficients of x in Eq. (5) can be obtained in several ways:

a) Use equations (1), (2), and (6) to calculate P and x, with U as a parameter. Fit the resulting values to Eq. (5) by least squares. This is the simplest procedure, but care must be taken to insure that the resulting curve goes through $P = 0$, $x = 0$. This can be done by weighting the (0,0) point very heavily.

b) If a suitable least squares program is not available, a fairly good determination of the coefficients can be made graphically through successive approximations, i.e. if (y,x) are the given values, proceed as follows:

i) plot y vs x and draw a straight line through the data. This gives

$$y_1 = \alpha x \tag{7}$$

ii) plot $y - y_1$ vs x^2 and again draw a straight line. The result is

$$y_2 = y_1 + \beta x^2 \tag{8}$$

etc.

This procedure works well for a parabola. Increasing care is required as higher order terms are introduced.

c) The coefficients in (5) may be determined analytically. With $P' \equiv dP/du$ and $u' \equiv du/dx$, the coefficients in (5) are

$$\alpha = \left.\frac{dp}{dx}\right|_{x=0} = (P'U')_{u=0} \tag{9.1}$$

$$\beta = \left.\tfrac{1}{2}\frac{d^2P}{dx^2}\right|_{x=0} = \tfrac{1}{2}(P''U'^2 + P'U'')_{u=0} \tag{9.2}$$

$$\gamma = \left.{}^1\!/_6\,\frac{d^3P}{dx^3}\right|_{x=0} = {}^1\!/_6(P'''U'^3 + 3P''U'U'' + P'U''')_{u=0} \tag{9.3}$$

$$\delta = \left.{}^1\!/_{24}\,\frac{d^4P}{dx^4}\right|_{x=0} = {}^1\!/_{24}(P^{iv}U'^4 + 6P'''U'^2U'' + 3P''U''^2 + 4P''U'U''' + P'U^{iv})_{u=0} \tag{9.4}$$

With P given by Eq. (2),

$$P_o' = \rho_o a, \quad P_o'' = 2\rho_o b, \quad P_o''' = 6\rho_o C, \quad P_o^{iv} = 24\rho_o d, \tag{10}$$

where

$$P_o' = (P')_{u=0}, \quad \text{etc.}$$

Values of U_o', U_o'', etc. are obtained by successive differentiations of the mass jump condition, as in Appendix A. With U_S given by Eq. (1), these are

$$U_o' = a \qquad U_o'' = 2a(b - 1) \tag{11.1}$$

$$U_o''' = 6a[(b - 1)^2 + ac] \tag{11.2}$$

$$U_o^{iv} = 24a[(b - 1)^3 + 3ac(b - 1) + a^2d] \tag{11.3}$$

Substitution of Eqs. (10) and (11) into Eq. (9) gives

$$\alpha = \rho_o a^2 \quad (12.1)$$

$$\beta = \rho_o a^2(2b - 1) \quad (12.2)$$

$$\gamma = \rho_o a^2[(b - 1)^2 + 2b(b - 1) + 2ac] \quad (12.3)$$

$$\delta = \rho_o a^2[(b - 1)^3 + 3b(b - 1)^2 + 6ac(b - 1) + 2abc + 2a^2d] \quad (12.4)$$

Determination of the coefficients of a power series in this fashion is often less satisfactory than least square fitting or alternative analytic methods. In this case the function fits very well near $x = 0 = u$, but falls off toward the upper range of validity of Eq. (2). This is shown in the following table, where coefficients for fused quartz have been used.

TABLE I

Analytical Fit to P(x) for Eqs. (1)-(6) for Fused Quartz

$a = 0.59755$ $b = -3.3398$ $c = 45.132$ $d = -188.88$ $\rho_o = 2.204$

$\alpha = 0.786973$ $\beta = -6.04364$ $\gamma = 80.0818$ $\delta = -1013.38$

U cm/μsec	U_S cm/μsec	x	P_1 kbar	P_2 kbar
.001	0.59426	0.168561×10^{-2}	1.30973	1.30973
.01	0.56848	1.79058×10^{-2}	12.5292	12.5092
.02	0.54730	3.79293×10^{-2}	24.1247	23.4272
.03	0.532875	5.96569×10^{-2}	35.2336	29.6064
.04	0.52408	8.26308×10^{-2}	46.2029	21.7012

P_1 is calculated using Eqs. (1), (2), (4), and (6).

P_2 is calculated from Eqs. (5) and (12).

The above constants give P in megabars with U_p and U_s in cm/μsec, ρ_o in g/cc.

2. When U_S and U_P are linearly related, the relation between P and X or P and η can be obtained exactly from Eq (6).

$$U_S = \frac{U}{\eta} = a + bu \quad (13.1)$$

$$u = \frac{a\eta}{1 - b\eta} \quad (13.2)$$

$$P = \rho_o U_S U = \frac{\rho_o u^2}{\eta}$$

$$= \frac{\rho_o a^2 \eta}{(1 - b\eta)^2} \quad (14)$$

Let U_S deviate from linear dependence on U, say

$$U_S = a + bu + \psi(u) \quad (15)$$

Let

$$u = u_o + u_1 \quad (16)$$

where

$$u_o = \frac{a\eta}{1 - b\eta} \quad (17)$$

Then

$$P = \frac{\rho_o u^2}{\eta} = \frac{\rho_o}{\eta}(u_o^2 + 2u_o u_1 + u_1^2) \quad (18)$$

and

$$U_S = a + bu_o + bu_1 + \psi(u_o + u_1) = \frac{u_o + u_1}{\eta} \quad (19)$$

Because of Eqs. (13) and (19),

$$\frac{u_1}{\eta} = bu_1 + \psi(u_o) + \left.\frac{d\psi}{du}\right|_{u_o} u_1 + \cdots \tag{20}$$

$$u_1 = \frac{u_o\psi(u_o)}{a - u_o(d\psi/du)_o} \tag{21}$$

Substituting this into Eq. (18) and retaining only terms of first order in u_1 gives

$$P = \frac{\rho_o u_o{}^2}{\eta} + \frac{2\rho_o u_o{}^2\psi(u_o)}{\eta[a - u_o(d\psi/du)_o]} \tag{22}$$

where

$$\frac{\rho_o u_o^2}{\eta} = \frac{\rho_o a^2\eta}{(1 - b\eta)^2} \tag{23}$$

Eq. (23) represents a perturbation of the Hugoniot P-V curve from its normal form corresponding to a linear U_S-U_P relation. Again, taking fused quartz as an example

$$\psi(u) = cu^2 + du^3$$

$$(d\psi/du)_{u=u_o} = 2cu_o + 3du_o^2$$

Then Eq. (22) becomes

$$P_2 = \frac{\rho_o a^2\eta}{(1 - b\eta)^2} + \frac{2\rho_o u_o^4(c + du_o)}{\eta(a - 2cu_o^2 - 3du_o^3)} \equiv P_2^{(0)} + P_2^{(1)} \tag{24}$$

TABLE II

Perturbation Hugoniot for Fused Quartz

Same Constants as Table I. P_1 from Table I

x	P_1	$P_2^{(\ )}$	$P_2^{(\ )}$	P_2
0.168561×10^{-2}	1.30973	1.30953	1.97×10^{-4}	1.30973
1.79058×10^{-2}	12.5292	12.3497	0.17873	12.5285
3.79293×10^{-2}	24.1247	22.8425	1.2639	24.1064
5.96569×10^{-2}	35.2336	31.3909	3.7223	35.1132
8.26308×10^{-2}	46.2029	38.1415	7.62715	45.7687

This simple calculation produces a remarkably good fit, as seen in Table II. Even at 46 kbar the error is only slightly greater than one percent.

3. Modified Series Expansion

The success of the perturbation calculation described in the preceding section suggests a series expansion in the parameter

$$y = a\eta/(1 - b\eta) \tag{25}$$

With U_S given by Eq. (1), the mass jump condition, Eq. (6), becomes

$$(1 + z)q = z(A + Bq + Cq^2 + Dq^3) \tag{26}$$

where

$$z = by/a, \quad q = au, \quad A = a^2/b, \quad B = 1, \quad C = c/ab, \quad D = d/a^2b$$

Hugoniot pressure is now expressed as

$$P = \alpha'y + \beta'y^2 + \gamma'y^3 + \delta'y^4 \tag{27}$$

The coefficients α', β', γ', δ', are determined in the same manner as α, β, γ, δ in Section 2. The derivatives of q with respect to z are obtained from Eq. (26) in the manner described in Appendix A. The derivative of U with respect to y are obtained by a simple transformation. With

$u'_0 \equiv (du/dy)_{y=0}$, we have

$$u'_0 = 1, \qquad u''_0 = 0, \qquad u'''_0 = 6c/a, \qquad u^{iv}_0 = 24d/a \tag{28}$$

The coefficients in Eq. (27) are

$$\alpha' = \rho_0 a, \quad \beta' = \rho_0 b, \quad \gamma' = 2\rho_0 c, \quad \delta' = 2\rho_0(d + bc/a) \tag{29}$$

Pressures in fused quartz calculated from the same values of x used in Tables I and II are given in Table III. The result is considerably better than that obtained from expansion in x (p_2 of Table I), but not quite as good as obtained from perturbation calculation of Table II.

TABLE III

Hugoniot pressures calculated from Eqs. (27) and (29), kbars. Pressures in kilobars. $P_2^{(1)} \rightarrow P_2^{(4)}$ are the contributions of individual terms in Eq. (22). P_1 from Table I.

x	$P_2^{(1)}$	$P_2^{(2)}$	$P_2^{(3)}$	$P_2^{(4)}$	P_2	P_1
0.168561 E-2	1.31689	-7.4×10^{-3}	2.0×10^{-4}	-3×10^{-6}	1.30973	1.30973
1.79058 E-2	13.0753	-0.7255	0.1947	-3.2×10^{-2}	12.5128	12.5292
3.79293 E-2	25.630	-2.787	1.466	-0.467	23.842	24.1247
5.06569 E-2	37.293	-5.902	4.517	-2.092	33.8157	35.2336
8.26308 E-2	47.864	-9.723	9.55	-3.392	44.299	46.2029

APPENDIX A

APPENDIX A

Derivatives of Particle Velocity

The mass jump condition is

$$(1 + x)u = xU_S \tag{1}$$

where $x = (V_o/V) - 1$. Denote dU_S/du by U_S', du/dx by U'. Eq. (1) gives by successive differentiation,

$$u + (1 + x)u' = U_S + xU_S'u' \tag{2}$$

$$2u' + (1 + x)u'' = 2U_S'u' + x(U_S''u'^2 + U_S'u'') \tag{3}$$

$$3u'' + (1 + x)u''' = 3U_S''u'^2 + 3U_S'u'' + x(U_S'''u'^3 + 3U_S''u'u'' + U_S'u''') \tag{4}$$

$$= A + xB$$

where

$$A = 3U_S'' u'^2 + 3U_S'u''$$

$$B = U_S''' u'^3 + 3U_S''u'u'' + U_S'u'''$$

Continuing,

$$(1 + x)u^{iv} + 4u''' = A' + B + xB'$$

$$A' = 3U_S''' u'^3 + 9U_S''u'u'' + 3U_S'u'''$$

So,

$$(1 + x)u^{iv} + 4u''' = 3U_S''' u'^3 + 9U_S''u'u'' + 3U_S'u''' + U_S''' u'^3 + 3U_S''u'u'' + U_S'u''' + xB'$$

$$(1 + x)u^{iv} + 4u''' = 4U_S''' u'^3 + 12U_S'' u'u'' + 4U_S' u''' + xB' \qquad (5)$$

Values of the derivatives are required at $x = 0$ where $u = 0$. Denote these by subscript "o". Then,

from (2) $\quad u_o' = U_{So} \qquad (6)$

from (3) $\quad u_o'' = 2U_{So}' u_o' - 2u_o' = 2u_o'(U_{So}' - 1) \qquad (7)$

from (4) $\quad u_o''' = 3U_{So}'' u_o'^2 + 3u_o''(U_{So}' - 1) \qquad (8)$

from (5) $\quad u_o^{iv} = 4U_{So}''' u_o'^3 + 12U_{So}'' u_o' u_o'' + 4u_o'''(U_{So}' - 1) \qquad (9)$

With $\quad U_S = a + bu + cu^2 + du^3, \quad U_{So} = a, \quad U_{So}' = b, \quad U_{So}'' = 2c, \quad U_{So}''' = 6d,$

$$\left.\begin{aligned} &\text{Then,} \quad U_o' = a, \quad U_o'' = 2a(b - 1), \quad u_o''' = 6a(b - 1)^2 + 6a^2c, \\ &U_o^{iv} = 24a[(b - 1)^3 + 3ac(b - 1) + a^2 d] \end{aligned}\right\} \qquad (10)$$