LA-UR -93-1421

Los Alamos National Laboratory is operated by the University of California for the United States Department of Energy under contract W-7405-ENG-36

TITLE: EQUATION OF STATE FOR DETONATION PRODUCTS

AUTHOR(S): WILLIAM C. DAVIS, M-7 P952

SUBMITTED TO: 10th Detonation Symposium Boston Mass. on
July 12-16, 1993

DISCLAIMER

This report was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor any agency thereof, nor any of their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof.

By acceptance of this article, the publisher recognizes that the U.S. Government retains a nonexclusive, royalty-free license to publish or reproduce the published form of this contribution, or to allow others to do so, for U.S. Government purposes.

The Los Alamos National Laboratory requests that the publisher identify this article as work performed under the auspices of the U.S. Department of Energy.

MASTER

Los Alamos

Los Alamos National Laboratory
Los Alamos, New Mexico 87545

FORM NO. 836 R4
ST. NO. 2629 5/81

DISTRIBUTION OF THIS DOCUMENT IS UNLIMITED

EQUATION OF STATE FOR DETONATION PRODUCTS

William C. Davis
Los Alamos National Laboratory
Los Alamos, NM 87545

ABSTRACT

An equation of state for detonation products, with the usual form $p=p(v,E)$, is proposed. It allows independent calibration of the adiabatic gamma and the Grüneisen gamma, and gives them forms in agreement with recent theoretical studies. The equation of state is given by

$$p = \frac{E}{v}\left[k - 1 + F(v)\left\{1 + b\left(1 - \frac{E}{E'(v)}\right)\right\}\right]$$

where $F(v)$ drops from a finite value at small v to zero at large v, b is a constant, and $E'(v)$ is the specific internal energy on the principal isentrope. Its relationship to the polytropic gas equation of state $p = (E/v)(\gamma - 1)$ is easily seen, and it reduces to this form at large volume.

INTRODUCTION

Studies[1,2] of the equation of state of detonation products using statistical mechanics have provided new insights into the behavior of the products, and studies[3,4] of the interaction of the equations of hydrodynamics with the equation of state have provided new constraints for the equation of state. Experiments[5] have shown that data for calibration of an equation of state can be obtained. Many empirical fitting forms have been proposed earlier, but they do not represent these new developments. Here we suggest an empirical fitting form that gives the important features their proper form.

A basic premise of this work has been to accept the fact that designers will modify any equation of state to compensate for the errors in their computer codes and in their representation of the device being modeled. An equation of state form that has the right physical properties, particularly the sound speed or adiabatic gamma, will give reasonable results even when severely adjusted. The forms considered here have the property that the physical properties are correctly represented. They are easy to adjust, and detailed instructions for adjusting them are included. The underlying physical constraints are discussed, to help users see where modification may lead to nonphysical results. Computer codes for hydrodynamic problems need an equation of state of the form $p = p(E,v)$. The equations suggested here have that form.

The simplest equation of state that has been used successfully for detonation products is the polytropic gas form

$$p = (E/v)(k - 1)\,, \tag{1}$$

where p is the pressure, E is the specific internal energy, v is the specific volume, and $k = -(v/p)(\partial p/\partial v)_S$ is the adiabatic exponent. At low density k is 1.2 or 1.3 for ordinary detonation product gases and is equal to the ratio of the specific heats. At high density the same form is often used, with $k \sim 3$, and it works fairly well at densities near the CJ density for many explosives. When the energy of the explosive products is transferred to the inert components in the pressure region where k falls from its high value to its low value, the polytropic equation of state fails.

The polytropic equation of state can be modified to

$$p = (E/v)[k - 1 + F(v)] \tag{2}$$

where F(v) has the value 0 at large specific volume, so the equation of state assumes its proper form at low density, and increases monotonically as the specific volume decreases, approaching a constant value at small volume. This simple modification gives the proper behavior on the principal isentrope, the isentrope through the CJ point, but is not sufficiently flexible off that isentrope to fit data such as the velocities of overdriven detonations.

The required flexibility is achieved with the form

$$p = \frac{E}{v}\left[k - 1 + F(v)\left\{1 + b\left(1 - \frac{E}{E'(v)}\right)\right\}\right] \tag{3}$$

where b is a constant and E'(v) is the specific internal energy on the principal isentrope. The parenthesis multiplied by b is zero on the principal isentrope, and the form is that of Eq(2). The bracket multiplied by b decreases the value of F(v) on isentropes above the principal isentrope, describing products that behave more like an ideal gas at a higher temperature, and increases the value for lower isentropes. The simple form for this term is consistent with the assumption that the region of interest for an equation of state for detonation products is always near the principal isentrope.

DEVELOPMENT

Now let us proceed to develop the expressions for the important physical quantities. The Grüneisen gamma

$$\Gamma = -\frac{v}{T}\left(\frac{\partial T}{\partial v}\right)_S = \frac{v}{T}\left(\frac{\partial p}{\partial S}\right)_v = v\left(\frac{\partial p}{\partial E}\right)_v \quad , \tag{4}$$

describes the variation of temperature along an isentrope, or the separation of isentropes with different internal energy at a constant volume. The adiabatic gamma

$$\gamma = -\frac{v}{p}\left(\frac{\partial p}{\partial v}\right)_S = \frac{v}{p}\,\frac{p + \left(\frac{\partial E}{\partial v}\right)_p}{\left(\frac{\partial E}{\partial p}\right)_v} = \frac{c^2}{pv} \tag{5}$$

is the non-dimensional sound speed, and describes the transport of energy by compression and rarefaction waves. These two quantities are the only[3,4] features of the equation of state that enter directly into the differential equations of hydrodynamics. It is important that their behavior is properly represented.

The equation of state is

$$p = \frac{E}{v}\left[k - 1 + F(v)\left\{1 + b\left(1 - \frac{E}{E^s(v)}\right)\right\}\right] \tag{6}$$

On the principal isentrope, where $E = E^s$, we have

$$p^s = (E^s/v)(k - 1 + F) \tag{7}$$

and by straightforward differentiation, using the fact that on an isentrope $dE/dv = -p$, we find that

$$\gamma^s = k + F - \frac{vF'}{k - 1 + F} \tag{8}$$

where $F' = dF/dv$. Notice that F' is negative, so the last term in the expression for γ' may make γ' have a maximum. Now from the definition of γ we see that

$$\int \frac{dp'}{p'} = -\int \gamma' \frac{dv}{v} = -\int \frac{k\,dv}{v} - \int \frac{F\,dv}{v} + \int \frac{dF}{k - 1 + F} \quad . \tag{9}$$

From the integration we obtain $p'(v)$, and by substitution into Eq(7) we find $E'(v)$ as

$$E'(v) = p'v/(k - 1 + F) \quad . \tag{10}$$

If we integrate Eq(9) from a chosen volume v_0 to an arbitrary volume v, and substitute the result into Eq(10), we find

$$\frac{E'(v)}{E'(v_0)} \quad \left(\frac{v_0}{v}\right)^{k-1} \exp\left(-\int_{v_0}^{v} \frac{F(v)\,dv}{v}\right) \quad . \tag{11}$$

The polytropic gas has the exponential term equal to zero, that is, $F(v) = 0$, and the energy on the isentrope varies as an inverse power of the volume. With $F(v) \neq 0$, the specific internal energy on the isentrope increases more rapidly as the volume is reduced.

The same differentiation of the general equation of state gives the expression for $\gamma(E,v)$ everywhere as

$$\gamma(E,v) = \gamma' + bF\left(1 \quad \frac{E}{E'}\right)\left[1 \quad \frac{1 \quad \frac{vF'}{F}}{E/pv} \quad \frac{E}{E'} \quad 1 \quad \frac{p'E}{pE'} \quad \frac{E}{E'}\right] \tag{12}$$

where $p = p(E,v)$ and $p' = p'(E',v)$

Similarly we find

$$\Gamma(E,v) \quad k \quad 1 + F\left[1 + b\left(1 \quad \frac{2E}{E'}\right)\right] \quad . \tag{13}$$

and

$$\Gamma'(E'\,v) \quad k \quad 1 + F(1 \quad b) \tag{14}$$

Notice here that choice of the constant b makes it possible to choose the value of Γ at small specific volume independent of the value of γ.

For shock stability and monotonicity of the Hugoniot curve in the p u plane we must have

$$\gamma \quad \Gamma \quad 1 \tag{15}$$

On the isentrope, this can be seen to be true from Eqs. (8) and (14), since $F'(v) < 0$, as long as $b > 0$.

The fundamental derivative of gas dynamics[3,4], which measures the convexity of isentropes and must be positive everywhere for ordinary detonation products, is given by

$$\mathcal{G} = \tfrac{1}{2}[\gamma + 1 - (v/\gamma)(\partial\gamma/\partial v)_S] \quad . \tag{16}$$

$\mathcal{G}$ can be easily found by differentiating γ.

The material velocity on an isentrope is found by integrating the Riemann equation

$$du/dp = \pm (v/\gamma p)^{1/2} \tag{17}$$

This equation cannot be integrated in closed form for useful choices of F(v). It must be integrated numerically.

The temperature and specific heats are not represented accurately by a simple equation of state of the kind proposed here. The evaluation of their values may be useful because a zero or a pole in T or C_V would indicate a serious flaw in the equation of state. The temperature on an isentrope is found[6] by integrating the differential equation

$$(v/T)(\partial T/\partial v)_S = -\Gamma \tag{18}$$

The specific heat at constant volume is found in a similar way from the differential equation[3]

$$(v/g)(\partial g/\partial v)_S = \Gamma + 1 - \gamma - (\Gamma p/g)(\partial\Gamma/\partial p)_v \quad . \tag{19}$$

where $g = pv/C_VT$. The ratio of specific heats[3] $C_p/C_V = \gamma/(\gamma - \Gamma^2/g)$ can be found once g is known.

EXAMPLE: A SIMPLE CHOICE FOR F(v)

A simple form for F(v) that has appropriate properties is

$$F(v) = 2a(v/v_0)^{-n}/[(v/v_0)^{n} + (v/v_0)^{-n}] \quad . \tag{20}$$

where a, n, and v_* are constants to be determined in the calibration of the equation of state. For large v, F = 0; for small v, F = 2a; and $F(v_*) = a$. F(v) is a smeared out step function; the constant a determines the height of the step, v_* the volume where the rise is half the total rise, and the exponent n the steepness of the rise. For use in the expressions developed above we need the derivative of F(v). It is easy to show that

$$vF' = -\frac{4an}{\left[\left(\frac{v}{v_*}\right)^{n} + \left(\frac{v}{v_*}\right)^{-n}\right]^2} \tag{21}$$

This value can be substituted into Eqs(18) and (12) for γ.

To integrate γ to find an expression for the principal isentrope we need the value of the integral

$$\int \frac{F}{v}dv = \ln\left[\frac{\left(\frac{v}{v_*}\right)^{n}}{\left(\frac{v}{v_*}\right)^{n} + \left(\frac{v}{v_*}\right)^{-n}}\right]^{a/n} . \tag{22}$$

Using the expressions developed above, we can now write the expression for the principal isentrope as

$$\frac{p'}{p_*} = \frac{\left[\frac{1}{2}\left(\frac{v}{v_*}\right)^{n} + \frac{1}{2}\left(\frac{v}{v_*}\right)^{-n}\right]^{a/n}}{\left(\frac{v}{v_*}\right)^{k+1+a}} \; \frac{k-1+F}{k-1+a} . \tag{23}$$

In this expression, p_* is a constant to be determined in the calibration. The value for p' is to be substituted into the equation of state to determine E'.

Although the thermal properties of the equation of state play no part in hydrodynamics calculations, it is is instructive to take a brief look at some of them. The temperature is obtained by integrating eq(18) to get

$$\frac{T'}{T_*} = \frac{\left[\frac{1}{2}\left(\frac{v}{v_*}\right)^{n} + \frac{1}{2}\left(\frac{v}{v_*}\right)^{-n}\right]^{(a/n)(1-b)}}{\left(\frac{v}{v_*}\right)^{k-1+a(1-b)}} \tag{24}$$

Notice that as v becomes very large, the right hand side reduces to $(v/v_*)^{-(k-1)}$, the expected value at low density. Notice also, however, that if b = 1, it has this value for all values of the density. The value of b, which does not affect the pressure along the isentrope, has a strong effect on the temperature.

It is also possible to use the expressions for p′ and T′ to see how pv/RT varies along the isentrope. We find

$$\frac{\frac{p'}{p_c}\frac{v}{v_c}}{\frac{T'}{T_c}} = \frac{\left[\frac{1}{2}\left(\frac{v}{v_c}\right)^{n} + \frac{1}{2}\left(\frac{v}{v_c}\right)^{-n}\right]^{ab/n}}{\left(\frac{v}{v_c}\right)^{ab}} \cdot \frac{k-1+F}{k-1+a} . \qquad (25)$$

The values of this function are

$$\frac{\frac{p'}{p_c}\frac{v}{v_c}}{\frac{T'}{T_c}} = \begin{cases} (k-1)/[2^{ab/n}(k-1+a)] & \text{for } v \to \infty \\ 1 & \text{for } v = v_c \\ (k-1+2a)/[2^{ab/n}(k-1+a)](v/v_c)^{-2ab} & \text{for } v \to 0 \ . \end{cases} \qquad (26)$$

Notice that if b = 0 the function reaches a finite value as v becomes small, and becomes large for other values of b. It always reaches a constant value for large v, as expected, where pv/RT = 1.

CALIBRATION ON THE PRINCIPAL ISENTROPE

The constraints on an equation of state are (1) the principal isentrope must pass through the CJ point; (2) the principal isentrope must be tangent to the Rayleigh line at the CJ point; (3) the work done at a chosen truncation volume must be simply correlated with the Gurney energy; (4) the work done at complete expansion must be equal to the total chemical energy; (5) the adiabatic gamma at large expansion must be that of the product gases when they behave as ideal gases. These five constraints allow the calibration of five constants in the equation of state.

Constraints (1) and (2) lead to the equations

$$v_j/v_0 = \gamma_j/(\gamma_j+1) \qquad (27)$$

$$p_j = \rho_0 D^2/(\gamma_j+1) \qquad (28)$$

where the subscript j indicates values at the CJ point, so v_j, p_j, and γ_j are values of these quantities at the CJ point, ρ_0 is the initial density of the explosive and v_0 is its reciprocal, the initial specific volume, and D is the detonation velocity. The density ρ_0 is known from measurement. D may be known from measurement, or may be estimated using one of several rules. If p_j has been measured, γ_j may be calculated from the equation above. More often p_j is not known. In this case, γ_j may be estimated from the empirical relationship

$$\gamma_j = 1.6 + 0.8\,\rho_0 \qquad (29)$$

or another similar relationship. The usefulness of an equation of state for most engineering calculations is not much affected by small errors in the CJ values. The tangency requirement, however, must be satisfied.

The Gurney energy is a measure of the energy available from the explosive to drive metal. In most applications, little energy is imparted to the metal after the pressure has fallen to 0.1 GPa, so the desired calibration quantity is the available energy between the CJ point and the volume at which the pressure on the isentrope is 0.1 GPa. The iteration to obtain this volume exactly is tedious, and it has been found satisfactory to assume the cutoff volume to be $7v_0$ instead of calculating an exact value. Figure 1 shows the Fickett-Jacobs diagram[8] with the area that will correspond to the Gurney energy shaded. The Gurney energy is obtained from a cylinder test or a dent plate test. The cylinder at 19-mm expansion has a volume expansion of about 7; the energy is given as E_{19}. Standard practice is to measure the apparent wall velocity u_{19} in mm/μs, and express the energy as $E_{19} = \frac{1}{2}u_{19}^2$, with units of $(\text{mm}/\mu\text{s})^2$ or kJ/g. The Gurney energy, with units of kJ/cm^3, is

$$e_g = E_{19}(M/V)[1 + \tfrac{1}{2}\rho_0/(M/V)] \qquad (30)$$

where M is the mass per unit length of the copper tube, usually 19.501 g/cm, V is the volume of the tube per unit length, usually 5.067 cm^3/cm, and ρ_0 is the initial density of the explosive. Lower case e is used because the upper case E is used for specific energy, or energy per unit mass; e means energy per unit volume, and has dimensions of pressure. It is obtained by multiplying E by the initial density, that is, $e_g = \rho_0 E$. The Gurney energy may also be obtained from the standard dent plate test, where, in units of kJ/cm^3,

$$e_g = (\text{dent}/\text{refdent})(1 + \rho_0/\rho_{ref})(1 + 4\rho_{ref}/\rho_0) \tag{31}$$

with dent equal to the measured dent in inches, refdent a constant equal to 0.510, and ρ_{ref} a constant equal to 1.250 g/cm^3.

The shaded area of the Fickett-Jacobs diagram is

$$[E(p_j,v_j) - \tfrac{1}{2}p_j(v_0 - v_j)] - E(p_7,7v_0) \tag{32}$$

where p_7 is the pressure on the isentrope at volume $7v_0$. A useful calibration rule is to make

$$1.115E_g = [E(p_j,v_j) - \tfrac{1}{2}p_j(v_0 - v_j)] - E(p_7,7v_0) \tag{33}$$

where the empirical factor 1.115 has been determined[9] from experiment. This equation assures that constraint (3) is approximately satisfied.

The chemical energy of the explosive is obtained by assuming the composition of the products at expansion to one atmosphere, and calculating the energy released as the explosive molecule transforms to those products. For ordinary CHNO explosives the products are usually assumed to be N_2, H_2O, CO_2, and C. The H_2O is assumed to be vapor at 100 C. The total area of the Fickett-Jacobs diagram is set equal to the chemical energy, as

$$E_0 = E(p_j,v_j) - \tfrac{1}{2}p_j(v_0 - v_j) \tag{34}$$

where E_0 is the chemical energy, satisfying the fourth constraint. This notation is correct, and E_0 is the energy at the initial state before detonation. The usual convention is followed here, with the energy of the products set to zero at expansion down the principal isentrope to one atmosphere. For calibration, to get energy per unit volume, we write $e_0 = \rho_0 E_0$.

The explosive product gases are N_2, H_2O, CO_2, CO, and some solid carbon. We assume that a reasonable value for the adiabatic gamma is obtained with k = 1.3. With this assumption, there are five constraints to determine the five parameters, a, k, v, p, and n of the assumed form for the equation of state.

To summarize, the four equations to solve simultaneously are

$$\gamma_j = k + F_j + \frac{4an}{(k-1+F_j)G_j^2} \tag{35}$$

$$p_j = p_c \cdot \frac{k-1+F_j}{k-1+a} \cdot \frac{(\frac{1}{2}G_j)^{a/n}}{(v_j/v_c)^{k+a}} \tag{36}$$

$$\rho_0 E_0 = \frac{p_j(v_j/v_0)}{k-1+F_j} - \tfrac{1}{2}p_j(1 - v_j/v_0) \tag{37}$$

$$\rho_0 E_0 - 1.115e_g = \frac{p_7(v_7/v_0)}{k-1+F_7} \tag{38}$$

where

$$F = \frac{2a(v/v_c)^{-n}}{(v/v_c)^n + (v/v_c)^{-n}} \tag{39}$$

$$G = (v/v_c)^n + (v/v_c)^{-n} \tag{40}$$

$$v_7 = 7v_0 \tag{41}$$

$$p_7 = p_c \cdot \frac{k-1+F_7}{k-1+a} \cdot \frac{(\frac{1}{2}G_7)^{a/n}}{(v_7/v_c)^{k+a}} \tag{42}$$

and the subscripts j and 7 on F and G indicate the volume to be used in the expression.

Some values chosen for calibration input, some derived quantities, and the values for the calibrated parameters are given in Table I. The values chosen for input are believed to be in reasonable agreement with available experimental results, but this paper is not the place for a review of the experiments. The value for k, although listed with the calibrated parameters, was fixed at 1.3 as stated above.

CALIBRATION OFF THE PRINCIPAL ISENTROPE

To calibrate the equation of state off the principal isentrope, which really means determining a value for the constant b, there must be data available that sample the behavior of the explosive off the principal isentrope. For some explosives, detonation velocities for overdriven detonations have been measured[7]. These measurements sample the high pressure branch of the detonation Hugoniot curve.

The detonation Hugoniot curve is given by

$$E - E_0 = \tfrac{1}{2} p (v_0 - v) \ . \tag{43}$$

The equation of state is

$$p = \frac{E}{v}\left[k - 1 + F(v)\left\{1 + b\left(1 - \frac{E}{E'(v)}\right)\right\}\right] \ . \tag{44}$$

These two equation must be solved simultaneously to obtain p(v) and E(v) on the detonation Hugoniot curve. A simple approach is to eliminate p from the equation of state by using the Hugoniot relation, which then gives a quadratic equation for E. The solution is

$$E = \frac{\epsilon}{2}\left[\left\{(\alpha - \beta)^2 + 4\alpha\frac{E_0}{\epsilon}\right\}^{1/2} - (\alpha - \beta)\right] \tag{45}$$

where $\alpha = 2v/(v_0 - v)$, $\beta = k - 1 + F(1 + b)$, and $\epsilon = E'/Fb$. The result for E is substituted into the equation of state to get p. The detonation velocity D is obtained from the Rayleigh line equation

$$D = \sqrt{\frac{p v_0^2}{v_0 - v}} \ . \tag{46}$$

The particle velocity u is obtained from the jump condition

$$u = \sqrt{p(v_0 - v)} \tag{47}$$

Fits to the data of reference 7, shown in Figs. 2 and 3, were obtained by eye rather than with the use of a least squares code. The values for b are given in Table I. The lowest point on the curves in Figs. 2 and 3, where there is a horizontal tangent, is fixed by the choice of a value for the detonation velocity. The tangent point is fixed in the horizontal direction by the choice for the CJ pressure, which in turn fixes the CJ particle velocity. Changing the constant b moves the left end of the curve in the high velocity region. For these reasons, the curves do not fit the data as well as they might if there were freedom to make them fit only these data.

With the assumption that the detonation is really exactly a CJ detonation, it can be shown[10] by differentiating the Hugoniot curve and the Rayleigh line with respect to initial state values, that

$$\frac{\rho_0}{D}\frac{dD}{d\rho_0} = \frac{\gamma - 1 - \Gamma}{2 - \Gamma/\gamma} \quad , \tag{48}$$

with Γ and γ evaluated at the CJ state. For PBX-9404, measured values of detonation velocity at different densities give a value of about 0.69 for this function. The calibration of this equation of state gives, at the CJ state, $\gamma = 2.991$ and $\Gamma = 0.853$. Substituting these values into the equation above gives 0.664 for the function. The disagreement is in keeping with the results discussed in ref. 10 and 11, where it was shown that the derivatives at the CJ state obtained from the simple theory did not agree with experiment. The fit to the velocities for overdriven detonations does not depend on derivatives nor on the CJ assumption, and the value of Γ found from them is to be preferred over one found from the variation of velocity with density.

DISCUSSION

Plots of γ and Γ for PBX-9404 and LX-17 are shown in Figs. 4 and 5. The fit for Γ is monotone, while the fit for γ has a maximum. The value for n is higher for LX-17 than for PBX-9404, and as a result the maximum is more pronounced for LX-17.

The form of the function F(v), and the linear function (with parameter b) for states off the principal isentrope, were chosen to have the right number of constants to determine using the calibration procedure described for the usual data available. If more measurements are available, then more complicated functions can be used. In particular, if the equation of state were to be used as a fitting form for γ and Γ computed from a statistical mechanical treatment of intermolecular forces, the functions could be made more complicated for a better fit.

In engineering use, it is often necessary to change the equation of state a little to reproduce experiments. Usually adjustment of the constant used to multiply the Gurney energy in Eqs(31) and (36) and then recalibrating will be sufficient.

ACKNOWLEDGEMENTS

Drs. J. B. Bdzil, W. Fickett, M. S. Shaw, and R. Menikoff have all contributed important concepts to this work.

REFERENCES

1. M. S. Shaw, "A new simulation method for the efficient calculation of benchmarks for detonation products equations of state," Ninth Symposium (International) on Detonation, pp. 452-60, 1989.

2. F. H. Ree, "A statistical mechanical theory of chemically reacting multiphase mixtures: application to the detonation properties of PETN," J. Chem. Phys. **81**, 1251-63, (1984).

3. W. C. Davis, "Equation of state for detonation products," Eighth Symposium (International) on Detonation, pp. 785-795, 1985.

4. Ralph Menikoff and Bradley J. Plohr, "The Riemann problem for fluid flow of real materials," Rev. Mod. Phys. **61**, 75-130 (1989).

5. W. A. Bailey, R. A. Belcher, D. K. Chilvers, and G. Eden, "Explosive equation of state by the AWRE method," Seventh Symposium (International) on Detonation, pp. 678-85, 1981

6. W. Fickett and W. C. Davis, *Detonation*, University of California Press, Berkeley, 1979, pp. 121-124

7. L. Green, E. Lee, A. Mitchell, and C. Tarver, "The supra-compression of LX-07, LX-17, PBX-9404, and RX-26-AF and the equations of state of the detonation products", Eighth Symposium (International) on Detonation, pp. 587-595, 1985

8. Reference 6, pp. 35-38.

9. The empirical factor that relates the Gurney energy and the truncated Fickett Jacobs energy is the crucial parameter of the calibration. The value used in Eq(31) was obtained by computing the ratios for calibrated equations of state that have been found sufficiently accurate to be useful, for example, the JWL constants given in Table 8.7 of B. M. Dobratz and P. C. Crawford, LLNL Explosives Handbook, UCRL 52997 Change 2, 1985. Users may find it advisable to make small adjustments to the factor for particular applications.

10. Reference 6, pp. 69-74

11. W. C. Davis, B. G. Craig, and J. B. Ramsay, "Failure of the Chapman-Jouguet theory for liquid and solid explosives", Phys. Fluids **8**, 2169-82 (1965).

TABLE 1

Calibration Input

explosive	D - m/s	p_j - GPa	ρ_0 - kg/m^3	E_{19} - MJ/kg	e_0 - GJ/m^3
PBX-9404	8790	35.7	1844	1.620	10.78
LX-17	7630	26.0	1904	1.070	8.13

Derived Values

explosive	v_0 - m^3/kg	v_j - m^3/kg	v_γ - m^3/kg	γ_j	e_j - GJ/m^3
PBX-9404	5.423×10^{-4}	4.064×10^{-4}	37.96×10^{-4}	2.991	7.728
LX-17	5.252×10^{-4}	4.020×10^{-4}	36.76×10^{-4}	3.263	5.137

Calibrated Parameters

explosive	k	a	n	v - m^3/kg	p - GPa	b
PBX-9404	1.3	0.8067	1.4470	8.727×10^{-4}	3.376	0.62
LX-17	1.3	0.8767	1.8644	6.325×10^{-4}	5.511	0.65

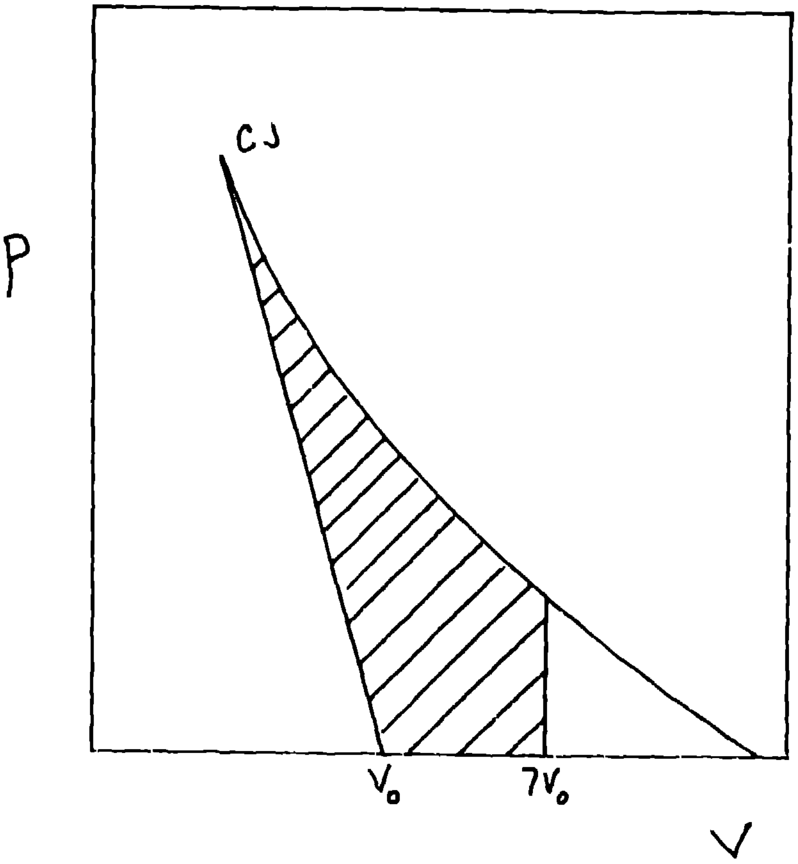

Fig. 1. The Fickett-Jacobs diagram of the quasistatic cycle for detonations. The total area of this diagram is approximately equal to the total energy of the explosive. The shaded area is the energy related to the Gurney energy. It represents the useful work done by the explosive driving an average metal system.

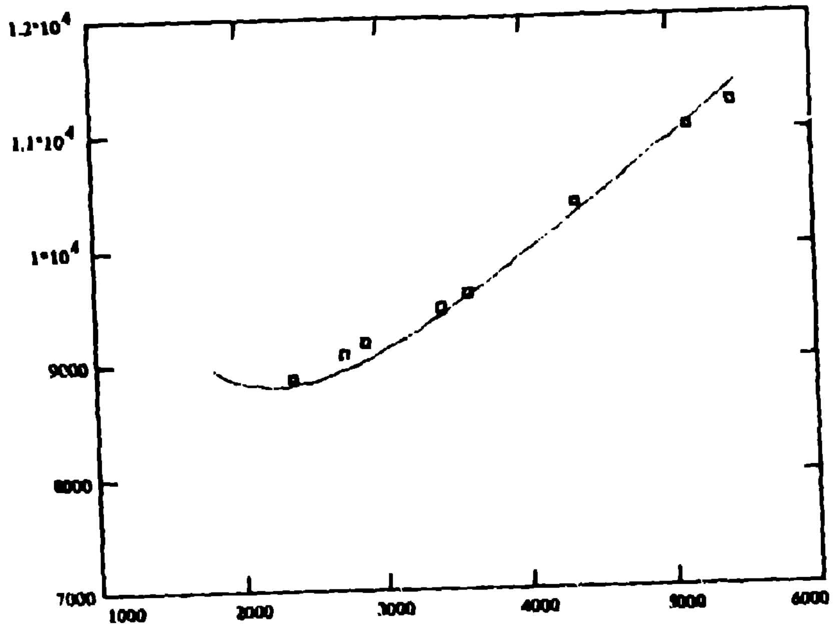

Fig. 2. Diagram in D-u space showing the data for overdriven detonation in PBX-9404 and the fit to the data used for calibration of the equation of state, with b = 0.62.

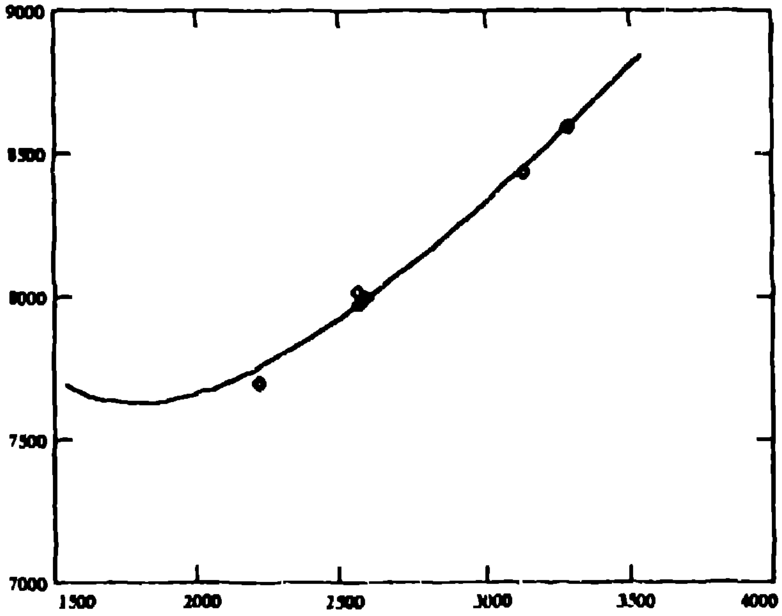

Fig. 3. Diagram in D-u space showing the data for overdriven detonation in LX-17, and the fit to the data used for calibration of the equation of state with b = 0.65.

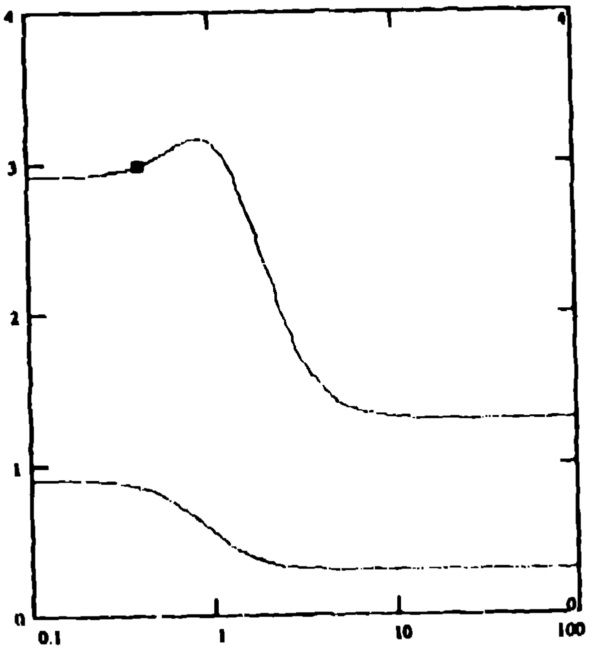

Fig. 4. Plot of γ and Γ vs log v for PBX-9404. The units of volume are cm^3/g. The CJ point is marked on the curve for γ.

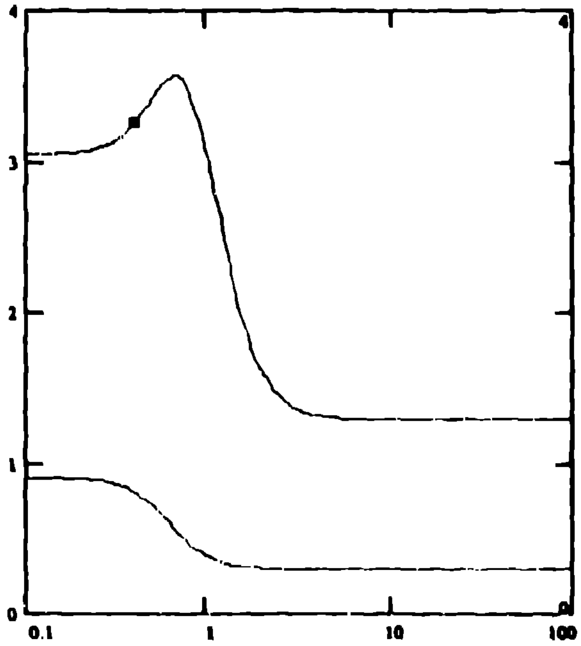

Fig. 5. Plot of γ and Γ vs log v for LX-17. The units of volume are cm^3/g. The CJ point is marked on the curve for γ.