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PARAMETRIC STUDY OF THE DYNAMIC JWL-EOS FOR DETONATION PRODUCTS*

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Abstract

The JWL equation of state describing the adiabatic expansion of detonation products is revisited to complete the description of the principal eigenvalue, to reset the secondary eigenvalue to produce a well-behaved adiabatic gamma profile, and to normalize the characteristic equation of state in terms of conventional parameters having a clear experimental interpretation. This is accomplished by interjecting a dynamic flow condition concerning the value of the relative specific volume when the particle velocity of the detonation products is zero. In addition, a set of generic parameters based on the statistical distribution of the primary explosives making up the available data base is presented. Unlike theoretical and statistical mechanical models, the adiabatic gamma function for these materials is seen to have a positive initial slope in accord with experimental findings.

Introduction

Equations of state of detonation products are mathematical expressions which characterize particle streamlines following the chemical reaction zone. They are used by research groups and laboratories to predict, simulate, and compare natural flow trajectories associated with energetic materials.

Presently, there are several renowned equations of state (EOS) for the detonation products. Each of these state equations was developed specifically to satisfy certain criteria and is used primarily by its originator. When it comes to choosing one EOS over another there are no clearly established rules. The choice usually is based on the ability to accommodate the algorithm into a computer program and its adaptability to desired changes and modifications. As an example, in his early review of compressibility of water, MacDonald(1) described four different polynomial and seven exponential equations of state that were applicable to solids and liquids. While demonstrating their usefulness he found none of them to be superior to any of the others.

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The Jones-Wilkins-Lee equation of state$^{(2-4)}$ (JWL-EOS) is an empirical mathematical expression used at this Laboratory and elsewhere to describe the pressure-volume relationship associated with chemical detonation products. It is used to calculate the state of the products as they expand from a certain high-pressure, high-density condition just after the chemical reaction to some terminal state at normal pressure and gaseous density. The JWL-EOS comprises two Murnaghan and one Tait equation of state. It represents pressure as a function of volume and energy P = P(V,E). In this normal form it satisfies the mechanics of the detonic flow problem but is incomplete for the thermodynamic description of the system and does not take into account explicit chemistry. The JWL is an EOS that is based on the Gruneisen principle but is fitted to experimental data. As with most other empirical equations of state, viscosity, conductivity, friction and body forces such as gravity are considered secondary effects. These transport properties are so small compared to the principal momentum of the system that they can easily be neglected.

The advantages of the JWL-EOS is its practical nature and the fairly large data base of experimental and popular explosives it supports. In addition, it is formulated on the basis of its two well-recognized predecessors: Murnaghan and Tait. However, after reviewing the literature on the subject and subjecting the JWL-EOS to a rigorous mathematical scrutiny, we recognized that the original set of coefficients and eigenvalues can be determined from well-defined boundary values associated with static and dynamic conditions. Thus, in revisiting the subject of the JWL-EOS it is the purpose of this communication to introduce a dynamic condition into the development of this equation which would not only eliminate guessing the principal eigenvalue but would also reduce the leading pressure coefficients to their primary dependents: the eigenvalues, the relative specific volume at the Chapman-Jouguet (CJ) plane, and the value of the reduced internal energy. This study will also reveal the small variance in governing parameters among various explosive systems. It will also show the effect of small changes in these parameters on the gamma profile, the most sensitive parameter of the detonic system.

The JWL-EOS

Parametric studies are usually carried out with normalized equations where all parameters appear in a nondimensional form. The JWL-EOS, as is familiar to all its users, is a mixed-dimensional equation, and for this study it must be brought into a normalized form. However, before doing that, let us first briefly review the relationship between various forms of this equation when the parameters and coefficients still represent dimensional quantities.

The most general form of the original JWL pressure algorithm, with all its boundary and initial (CJ) conditions appropriate to the dynamic detonic flow, is written as

$$P = A\left(1-\frac{\omega}{R_1 V}\right)e^{-R_1 V} + B\left(1-\frac{\omega}{R_2 V}\right)e^{-R_2 V} + \omega\frac{E}{V}: \tag{1}$$

This expression relates pressure P to the relative specific volume $V = v/v_0$ and energy E. Here, specific volume v_0 is the inverse of the initial density of the explosive, and the specific volume v is the independent variable. The energy term E contains chemical bond energy as well as kinetic energy associated with the momentum aspect of the flow. A, B, and C are the pressure coefficients, R_1 and R_2 are the principal and secondary eigenvalues, respectively, and ω is the fractional part of the normal Tait equation adiabatic exponent.

To simplify Eqn. 1 the energy dependance can be consolidated by imposing the restriction that the flow be adiabatic. Then, from the first law of thermodynamics,

$$dE = Tds - Pdv; \tag{2}$$

neglecting entropy changes, we find

$$dE = -Pdv. \tag{3}$$

As a consequence, this also means that the temperature T plays no significant role in characterizing the expansion process following the release of chemical energy within the reaction zone of the detonation wave.

Differentiating Eqn. 1, applying the restricting condition of Eqn. 3, and solving the resulting differential equation by quadrature, one can show that the usual isentropic form of the JWL-EOS becomes

$$P = Ae^{-R_1 V} + Be^{-R_2 V} + CV^{-(1+\omega)}, \tag{4}$$

where the two inside terms are Murnaghan expressions and the last term is the usual Tait expression. By integrating Eqn. 3, with Eqn. 4 substituted for P, one gets the expression for energy

$$E = \frac{A}{R_1}e^{-R_1 V} + \frac{B}{R_2}e^{-R_2 V} + \frac{C}{\omega V^{\omega}}. \tag{5}$$

The above expressions for pressure and energy are applicable along the isentropic release adiabat as well as at the initial CJ state point. In addition, by introducing the tangency condition at the CJ point where the isentrope is tangent to the Rayleigh line

$$\left(\frac{dP}{dV}\right)_{CJ} = -\rho_o D^2, \tag{6}$$

we can get a set of three equations (4, 5, and 6) which can be solved to determine the three pressure coefficients A, B and C:

$$A = \frac{R_1}{R_1 - R_2}\,\frac{P_c\left(1+\omega - \dfrac{V_c^2R_2^2}{\omega}\right) - E_c(1+\omega - V_cR_2)R_2 - \rho_oD^2V_c\left(1 - \dfrac{V_cR_2}{\omega}\right)}{1 + \omega - V_c(R_1 + R_2) + V_c^2R_1R_2/\omega}\,e^{R_1V_c}, \tag{7a}$$

$$B = \frac{R_2}{R_1 - R_2}\,\frac{-P_c\left(1+\omega - \dfrac{V_c^2R_1^2)}{\omega}\right) + E_c(1+\omega - V_cR_1)R_1 + \rho_oD^2V_c\left(1 - \dfrac{V_cR_1}{\omega}\right)}{1+\omega - V_c(R_1+R_2) + V_c^2R_1R_2/\omega}\,e^{R_2V_c}, \text{ and} \tag{7b}$$

$$C = \frac{-P_c(R_1+R_2) + E_cR_1R_2 + \rho_oD^2}{1 + \omega - V_c(R_1 + R_2) + V_c^2R_1R_2/\omega}\,V_c^{2+\omega}. \tag{7c}$$

Here the subscript 0 denotes initial conditions and the subscript c designates the Chapman-Jouguet state, which is a physically and mathematically acceptable transition point between a steady wave (the reaction zone) and the isentropic release wave, also known as the Taylor wave.

Up to this point all the expressions were written in the customary JWL mixed-dimensional form. To carry out our parametric study, these expressions must be transformed into a nondimensional format.

The most useful normalization factor is the "dynamic pressure," $\rho_o D^2$, (Eqn.6) which normalizes both pressure and energy. Thus, when so normalized all of the parameters become nondimensional and are designated with a tilde(~) above them; i.e.,

$$\tilde{F} = \frac{F}{\rho_o D^2}. \tag{8}$$

Transforming the isentropic JWL-EOS (Eqn. 4) into its nondimensional form, we get

$$\tilde{P} = \tilde{A}e^{-R_1 V} + \tilde{B}e^{-R_2 V} + \tilde{C}V^{-(1+\omega)}, \tag{9}$$

where coefficients A, B and C from Eqn. 7 become

$$\tilde{A} = \frac{R_1}{R_1-R_2}\,\frac{(1-V_c)\left(1+\omega-\dfrac{V_c^2R_2^2}{\omega}\right) - [1/2(1-V_c)^2 + \tilde{E}_o]\,(1+\omega - V_cR_2)R_2 - V_c\left(1-V_c\dfrac{R_2}{\omega}\right)}{(1+\omega) - V_c(R_1+R_2) + V_c^2R_1R_2/2}\,e^{R_1V_c}, \tag{10a}$$

$$\tilde{B} = \frac{R_2}{R_1-R_2}\,\frac{-(1-V_c)\left(1+\omega-\dfrac{V_c^2R_1^2}{\omega}\right) + \left[\dfrac{1}{2}(1-V_c)^2 + \tilde{E}_o\right](1+\omega - V_cR_1)R_1 + V_c\left(1-V_c\dfrac{R_1}{\omega}\right)}{(1+\omega) - V_c(R_1+R_2) + V_c^2R_1R_2/2}\,e^{R_2V_c}, \text{ and} \tag{10b}$$

$$\tilde{C} = \frac{1 - (1-V_c)(R_1+R_2) + \left[\dfrac{1}{2}(1-V_c)^2 + \tilde{E}_o\right]R_1R_2}{(1+\omega) - V_c(R_1+R_2) + V_c^2R_1R_2/2}\,V_c^{2+\omega}. \tag{10c}$$

During this transformation we have also made use of the nondimensional identities described earlier(5) for the CJ state, namely:

$$\tilde{P}_c = 1 - V_c \tag{11}$$

and

$$\tilde{E}_c = \tilde{E}_o + \tilde{P}_c(1-V_c)/2 = \tilde{E}_o + \tilde{P}_c^2/2, \tag{12}$$

where the energy value of the CJ state has been augmented by the flow condition and now represents the sum of the normal energy density and the kinetic energy.

These identities are the ordinary jump conditions. They allow us to suppress pressure dependency at the CJ plane by substituting pressure terms with the more important independent relative specific volume term V_c.

Two important features about the normalized JWL-EOS can be noted at this point:

- When Eqn. 9 is evaluated at the CJ point it must reduce to Eqn. 11. This means that the initial condition of the EOS is completely independent of energy, a point that will be verified later.

- The normalized pressure coefficients $\tilde{A}$, $\tilde{B}$, and $\tilde{C}$ depend not only on the two primary explosive parameters V_c and E_o but also on the entire set of eigenvalues R_1, R_2 and ω.

The values of V_c and $\tilde{E}_o$, along with their variances for the explosives taken from the available data base,(6) have already been established.(5) For thirty-one different explosives the values of V_c and $\tilde{E}_o$ are 0.7347±0.0065 and 0.0826±0.0125, respectively. For greater accuracy, the energy value can be considered density-dependent and can be written as $\tilde{E}_o = 0.204 - 0.0734\rho_o$.

The Eigenvalues

The beginning of the adiabatic expansion process for detonation products, initially accelerated into motion in the reaction zone, starts a deceleration phase at the CJ plane. These particles will quickly slow down, stop, and, depending on the rear boundary, will most likely reverse their direction as the products expand. For a point-initiated spherical wave, the particles are more likely to just stop. For cylindrical and plane waves, the particles will reverse their direction of motion. Thus, along a streamline there is a point at which the mass motion stops and the particle velocity is zero. This point in space and time provides an additional condition to determine the principle eigenvalue R_1 and in turn the remaining unknown quantities.

To utilize this additional state of zero particle velocity along the release streamline, we shall invoke the dynamic relationship between the principal detonic variables,(7,8) where, as before, the transport properties are neglected. This dynamic relationship can be written as:

$$\dot{P}\,\dot{v} + \dot{u}^2 = 0, \qquad (13)$$

where the dot above the symbols refers to total temporal differentials. After normalizing and rearranging of terms, we can write

$$\frac{u_c}{D} = 1 - V_c = \int_{V_c}^{V(u=0)} \sqrt{-(d\tilde{P}/dV)dV}, \qquad (14)$$

which represents conditions along a streamline involving detonic variables between the CJ plane and the location where the particle velocity is zero.

The utility of the above expression can be demonstrated by considering the classical case of the constant-gamma equation of state, PV^{Γ} = const, for which this integral can easily be evaluated to yield the expression

$$V(u=0) = \frac{1}{2}\left(\frac{2\Gamma}{\Gamma+1}\right)^{\frac{\Gamma+1}{\Gamma-1}}. \tag{15}$$

For the usual $\Gamma=3$ case, we find

$$V(u=0,\Gamma=3) = 9/8 = 1.125. \tag{16}$$

However, the JWL is not a constant-gamma EOS. It is designed to account for the gamma range between a certain value near 2.77 (Ref. 5) at the CJ plane and the adiabatic exponent of the final polytropic gaseous products. When the isentropic JWL-EOS (Eqn. 9) is substituted into Eqn. 14, there is no closed-form solution to the integral, and one must resort to a close approximation. There are several ways to approach the problem, among which are the Adams-Boshforth technique, the three-eights rule, or Simpson's method.(9) The latter was selected for this work after testing it for stability and accuracy. The method is described in more detail in the Appendix. In essence, the solution involves determining the approximate relative specific volume of the reacted products at the point where the particle velocity is zero and then iterating to a unique final value.

Such a procedure was followed to determine V(u=0) for all the explosives listed in the data base.(6) These values are given in Table 1 together with the corresponding values of ρ_0, D, V_c and E_0. Also shown in the Table are arithmetic averages with their respective variances and standard deviations. The results were both interesting and significant. For all listed explosives, the value of V(u=0) is nearly a constant $V_{ave}(u=0) = 1.1189+0.0050$, with a standard deviation not exceeding 0.5%. This observation allowed us to use this unique value of V(u=0) in the iterative process to solve for R_1 and R_2.

During this procedure an estimate had to be made of the relationship between the two eigenvalues R_1 and R_2.. One could either make an estimate of R_2 and treat it as a constant or establish R_2 as a function of R_1 and recompute its value during the iteration procedure. One could also require that R_2 serve some other specific purpose, such as matching a certain value of gamma with the value of V(u=0). This latter assumption would require justification and more extensive

Table 1. Selected properties of the major primary explosives.

Explosive	ρ (g/cc)	D (mm/μs)	V_{CJ}	$\tilde{E}_0$	$V(u_p = 0)$
BTF	1.859	8.480	0.730703	0.086025	1.12655
Comp A-3	1.650	8.300	0.736074	0.078297	1.11734
Comp B	1.717	7.980	0.730197	0.077739	1.11774
Comp C-4	1.601	8.193	0.739456	0.083746	1.11566
Cyclotol	1.754	8.250	0.731952	0.077063	1.11885
DIPAM	1.550	6.700	0.741303	0.089106	1.11969
EL-506A	1.480	7.200	0.732805	0.091237	1.11589
EL-506C	1.480	7.000	0.731108	0.085493	1.11431
Expl. D	1.420	6.500	0.733311	0.090007	1.1176
FEFO	1.590	7.500	0.720475	0.089447	1.12279
HMX	1.891	9.110	0.732378	0.066905	1.11629
HNS	1.400	6.340	0.742331	0.106621	1.12073
HNS	1.650	7.030	0.736340	0.091361	1.12002
LX-01	1.230	6.840	0.730651	0.106001	1.12648
LX-04-1	1.865	8.470	0.745883	0.071003	1.11407
LX-07	1.865	8.640	0.745010	0.071827	1.11392
LX-09-1	1.840	8.840	0.739199	0.073024	1.11853
LX-10-1	1.865	8.820	0.741526	0.071683	1.11697
LX-11	1.875	8.320	0.745747	0.069341	1.11197
LX-17-0	1.900	7.600	0.726636	0.062873	1.11146
NM	1.128	6.280	0.719015	0.114641	1.13192
Octol 78	1.821	8.480	0.738829	0.073311	1.11739
PBX-9010	1.787	8.390	0.729709	0.071547	1.11586
PBX-9011	1.777	8.500	0.735178	0.069320	1.11399
PBX-9404	1.840	8.800	0.740331	0.071584	1.11762
PBX-9407	1.600	7.910	0.735288	0.085906	1.12112
Pentolite	1.700	7.530	0.735453	0.084032	1.12116
PETN	1.500	7.450	0.735747	0.102818	1.13107
PETN	1.770	8.300	0.725264	0.082830	1.1259
Tetryl	1.730	7.910	0.736703	0.075755	1.11671
TNT	1.630	6.930	0.731734	0.089421	1.11598
average			0.734720	0.082579	1.118889
variance			0.000042	0.000155	0.000024
			0.01%	0.19%	0.00%
std. dev.			0.006536	0.012488	0.004989
			0.89%	15.12%	0.45%

programming for solving simultaneous differential equations. Therefore, for the purpose of this communication we have chosen the second estimate, which states that

$$R_2 = \kappa R_1 \tag{17}$$

where κ is a constant. This relationship is relatively easy to handle, and, judging from the existing data base,(6) it is also a very reasonable one. For most of the H-C-N-O explosives in the data base, $\kappa = 0.27$ with a standard deviation from an average of not more than 2%.

The final parameter value needed for the solution of Eqn. 14 is related to the ground-state adiabatic exponent γ. Of the three terms in the JWL-EOS (Eqn. 9), the third term containing ω dominates at the far end of the expansion; i.e., when the products approach some normal state at atmospheric conditions. Thus, the exponent $(1+\omega)$ represents the terminal value of the adiabatic exponent gamma, which for polytropic gases, such as the products of an explosive reaction, would be near the value of 4/3. This results in ω having the value of 1/3, the value chosen for the solution of Eqn. 14.

Thus, with all the unknowns in the Eqn. 14 either determined or properly estimated, the iterative process, although tedious, can easily be performed to yield a unique set of eigenvalues and coefficients required to carry out calculations with the JWL-EOS. These then, together with the results reported earlier,(5) form a complete set of characteristic values which fully describes a generic explosive in a nondimensional form. The list of these characteristic values is given in Table 2.

Table 2. List of characteristic values for a generic explosives.

$\tilde{P}_c = P_c/\rho_o D^2 = 0.2653$
$U_c = u_c/D = 0.2653$
$V_c = v/v_o = 0.7347$
$V(u{=}0) = 1.119$
$\Gamma_c = V_c/(1-V_c) = 2.77$
$\tilde{E}_o = E_o/\rho_o D^2 = 0.204 - 0.0734\rho_o$ or
$\tilde{E}_{oave} = 0.0826$

$\omega = \gamma - 1 = 1/3$
$\kappa = R_2/R_1 = 0.27$
$R_1 = 4.41604$
$\tilde{A} = A/\rho_o D^2 = 5.35545$
$\tilde{B}_o = B/\rho_o D^2 = 0.094983$
$\tilde{C} = C/\rho_o D^2 = 0.0112292$

Normally, the expansion of the detonation products is shown on the pressure-specific volume plane. However, the behavior of the products on this plane is always a monotonically decaying function with a very steep slope at the beginning. The release adiabat is therefore best illustrated by a profile of the system gamma, defined as

$$\Gamma \equiv -\frac{d\ln\tilde{P}}{d\ln V} \tag{18}$$

Both the normalized pressure and the system gamma curves are shown in Fig. 1 for our generic explosive whose characteristic values are listed in Table 2. In this figure the pressure curve drops quickly from its nondimensional CJ value of 0.2656 to less than 10% of that value at the relative specific volume of 1.6. Thereafter, the curve decays only gradually to some final normal state. The gamma function, on the other hand, forms a profile with a positive slope at the CJ point and two distinct humps during the expansion process. As we will see in the following sections, both humps can be controlled and varied but at a cost of loosing the validity of the experimental data which generated the original fitting process..

Effect of Internal Energy $\tilde{E}_o$

From the list of characteristic values for a generic explosive only one, the normalized energy - E_o, could not be stated as a constant. Rather, it turns out to be a simple linear function of the initial density.(5) To see the effect of this value on the products EOS it is best to look at the profile of the system gamma. This effect is illustrated in Fig. 2, where the value of $\tilde{E}_o$ is varied by ±12% from the average normalized value of 0.0826. The remaining variables which accompany this change are listed in Table 3 below

Table 3. Generic JWL-EOS coefficients with corresponding values of the relative energy

Constants unaffected by the change in $\tilde{E}_o$:

V_c = 0.7347
V(u=0) = 1.119
κ = 0.27
ω = 1/3

Curve in Fig. 2	$\tilde{E}_o$	R_1	$\tilde{A}$	$\tilde{B}$	$\tilde{C}$
1	0.0726	4.4298	5.4202	0.11103	6.621E-3
2	0.0826	4.4160	5.3555	0.09499	0.011229
3	0.0926	4.4025	5.2915	0.07909	0.015844

Figure 2 clearly shows that there is no effect on the initial CJ point for energy changes that are different from the generic value of $\tilde{E}_0$. Even in the central region of the plot, where the energy term is most effective in displacing the gamma profile, there is very little change. The effect of $\tilde{E}_0$ is reflected in the size of the second hump; i.e., the smaller $\tilde{E}_0$ of larger initial explosive density, the higher the second hump. The second hump may altogether vanish if the energy value is increased.

Although not directly associated with the energy term, Lee and Hornig(3) have studied the effect on the gamma profile by varying the loading density of PETN charges. If one takes into account the linear relationship between normalized energy and charge density,(5) then PETN results confirm our finding of the effect of $\tilde{E}_0$ on the shape of the gamma profile.

Effect of Relative Specific Volume V(u=0)

As mentioned earlier the value of V(u=0) controls the eigenvalue R_1. This is illustrated in Fig. 3 which shows the profile of gamma for three different values of V(u=0). The remaining coefficients corresponding to these three profiles are listed in Table 4.

Table 4. Generic JWL-EOS coefficients with corresponding values of the relative specific volume at zero particle velocity.

Constants unaffected by the change in V(u=0):

$V_c = 0.7347$
$\tilde{E}_0 = 0.0826$
$\kappa = 0.27$
$\omega = 1/3$

Curve in Fig. 3	V(u=0)	R_1	$\tilde{A}$	$\tilde{B}$	$\tilde{C}$
4	1.109	3.89695	4.43962	7.619E-4	0.0173148
2	1.119	4.41604	5.35545	0.094983	0.0112292
5	1.129	10.83395	88.59385	1.849790	0.0123951

Note: The large value of $\tilde{A}$ for Curve 5 shifts the whole waveform to the left, dropping off the usual first hump.

The sensitivity of this parameter is immediately evident. By varying the value of V(u=0) by less than 1% above and below the established generic value, we see a dramatic change in the profile of the system gamma. Also, both deviations (Curves 4 and 5) cause the gamma profile to loose its second hump and attain the normal state at a much higher density than the original generic case (Curve 2). By increasing the value of V(u=0), we also notice that the initial slope of gamma at the CJ point becomes negative. This condition is similar to statistical mechanical and other equations of state in general use. However, this negative initial slope of the gamma profile does not agree with experimental evidence, as will be shown later.

The Effect of Eigenvalue Ratio $\kappa = R_2/R_1$

While evaluating R_1 and R_2 it was postulated that they are related through a proportionality constant κ (Eqn. 17). The generic value of this constant was chosen on the basis of the existing data base.(6) However, this value may not be correct, and therefore one needs to know what effect this constant has on the gamma profile. Again, as before, the effect of κ is illustrated in Fig. 4 with all corresponding constants listed in Table 5.

Table 5. Generic JWL-EOS coefficients with corresponding values of the eigenvalue ratio κ.

Constants unaffected by the change in κ:

V_c = 0.7347
V(u=0) = 1.119
$\tilde{E}_0$ = 0.0826
ω = 1/3

Curve in Fig. 4	V(u=0)	κ	R_1	$\tilde{A}$	$\tilde{B}$	$\tilde{C}$
6	1.119	0.23	4.36546	5.30387	0.074540	9.9634E-3
2	1.119	0.27	4.41604	5.35545	0.094983	0.0112292
7	1.119	0.31	10.91562	55.58986	2.69632	0.0149773
8	1.109	0.23	3.98664	4.46918	6.202E-4	0.0173026
6	1.119	0.23	4.36546	5.30387	0.074540	9.9634E-3
9	1.129	0.23	4.78633	6.41625	0.150261	5.1677E-3

As is evident from Fig. 4a, raising the value of κ by about 15% produces the previously noted effect of enlarging the first hump, eliminating the second, and reaching its normal state isentropic gamma value at a much higher density. However, lowering the value of κ by 15% one can see almost no change in the gamma profile. At the lower κ the effect becomes evident when variation in V(u=0) is also introduced. This is seen in the adjacent Fig. 4b, where $\kappa = 0.23$ and V(u=0) is varied between 1.109 and 1.129. Here, depending on the value of V(u=0), the second hump of the gamma profile can be either greater or less than the first hump. Also, as in the other extreme cases, the second hump can disappear all together.

Slope of Gamma at the CJ Point

Completely independent of any EOS, the plane wave hypothesis is used to express the normalized system gamma as

$$\Gamma = \frac{V}{\tilde{P}}\left(\frac{dU}{dV}\right)^2 = \frac{V\left(\frac{X_c}{X}\right)^2}{1-V_c-\int_{V_c}^{V}\left(\frac{X_c}{X}\right)^2 dV} \tag{19}$$

where X is the location of the detonation front in Cartesian coordinates with the origin placed at the surface of initiation, X_c is the specific location of the CJ plane that is on the same streamline along which the particle velocity is being considered, and U is the normalized particle velocity. We emphasize that the above expression is EOS-independent and applies to all plane-wave detonic systems whether they are steady, self-similar, or isentropically expanding.

The relationship between V and X/X_c is quite complex, since it involves not only the streamline position but also the particle velocity. Nevertheless, near the CJ point this relationship can be simplified by letting the dynamic motion be sufficiently small that the positional ratio can be considered unity. Then, in the near proximity of the CJ plane, we get

$$\Gamma_{V_c \leq V << 1} = \frac{V}{1-V} \tag{20}$$

and the initial slope can be expressed as

$$\frac{d\Gamma}{dV} = \frac{1}{(1-V)^2} \tag{21}$$

which is positive because any increase in V will lead to an increase in Γ.

Summary

The present list of known explosives has a fairly large data base. Examining the data base, we noted that when each listing was normalized by its dynamic pressure, $\rho_0 D^2$, all available

H-C-N-O type explosives statistically converged to a single generic prototype, whose characteristic values are listed in Table 2. This generic explosive can then be used to fully describe the behavior of any new material when only the values of initial density (ρ_o) and detonation velocity (D) are available.

The products equation of state describes the isentropic expansion of the reaction products from their initial CJ state to some terminal state at atmospheric pressure and gaseous density. Among the currently popular equations of state used to describe expansion of the detonation products, the JWL-EOS was found to be the most practical and descriptive.

Although the JWL-EOS was originally proposed as an experimental EOS requiring a certain amount of fitting to experimental data , the normalization procedure and the introduction of an additional dynamic condition for the specific volume at the state where particle velocity is zero revealed that all characteristic values in a nondimensional form are either unique or interrelated to such an extent that very little or no guessing at all is necessary to fill the complement of parameters and coefficients needed to evaluate the algorithm. The list of nondimensional values pertaining to the generic explosive should be sufficient to describe the behavior of any explosive and in particular the behavior of the reaction products.

The three terms making up the JWL-EOS control the whole adiabatic expansion region, and that control is reflected in the shape of the gamma profile. The principal eigenvalue R_1 dominates the wave shape at and near the beginning of the gamma profile near the CJ plane . Its dominance extends to about where particle velocity becomes zero. Following this region the secondary eigenvalue R_2 along with the energy value $\widetilde{E}_o$ controls the transition region before the adiabatic exponent takes over. The energy value $\widetilde{E}_o(\rho_o)$ depends on the initial density, ρ_o, but does not influence initial CJ conditions. However, the value of energy does affect the size and shape of the second hump in the gamma profile. Together with the value of R_2, the energy value can be used to eliminate the second hump altogether, if it is deemed objectionable. In the present analysis we selected the secondary eigenvalue to be linearly dependent on the primary eigenvalue to preserve the waveform shapes of the existing data base. After the second hump the gamma profile asymptotically approaches the atmospheric state at some very large expansion. For this work the state chosen is the usual one described by the adiabatic exponent associated with a polytropic gas.

The gamma profile for the materials making up the published JWL-EOS data base has an initial positive slope starting at the CJ plane. To our knowledge no other equation of state follows this description. Rather, they all start out in a negative direction and monotonically decay to some atmospheric condition. Very little experimental evidence supports this positive slope contention, but what is available does confirm the plane wave theoretical evidence. For this reason it is deemed desirable, notwithstanding statistical mechanical results to the contrary, to implement JWL equation of state which supports these limited observations, as opposed to nondynamic equations of state, which concern only pressure-volume conditions.

At the present state of our understanding, the second hump of the gamma profile has no apparent reality. It is still an artifact of the old curve-matching technique that required a particular pressure-volume relationship. This hump is still present with the description of the generic explosive. However, one should bear in mind that its existence is not absolute, and it can be eliminated by a proper choice of energy $\tilde{E}_0$ and secondary eignevalue without affecting other characteristic features of the expansion.

From Tables 3, 4 and 5 one should also notice two distinct regions of the primary eigenvalues: those around 4.4 and those around 10. The former result in the familiar gamma profile with the double humps while the latter have no second hump. This change to high values affects the initial slope at the CJ plane even to the extent that a negative initial slope is a distinct possibility. This type of profile decays much more rapidly and attains the value of polytropic gamma at significantly higher densities.

In most respects, the JWL-EOS is a well-behaved expression ranging over a wide choice of gamma profile features. It is well-identified by Murnaghan and Tait, and above all it conforms to theoretical expectations for plane waves and experimental observations that the slope of the gamma function for the expanding products at the CJ plane is positive.

Appendix

After invoking the dynamic relationship among the principal detonic variables

$$\dot{P}\dot{v} + \dot{u}^{2} = 0 \tag{A-1}$$

and normalizing it with the dynamic pressure, $\rho_0 D^2$, we arrive at Eqn. 14 in the text:

$$\frac{u_c}{D} = 1 - V_c = \int_{V_v}^{V(u=0)} \sqrt{-(d\tilde{P}/dV)dV} \tag{A-2}$$

This equation represents the condition under which one can evaluate the relative specific volume at the state where the particle velocity is zero.

Taking the derivative of Eqn. 9 and substituting it into Eqn. A-2, we get

$$1-V_c = \int_{V_c}^{V(u=0)} \left[R_1\tilde{A}e^{-R_1 V} + R_2\tilde{B}e^{-R_2 V} - \frac{1+\omega}{V^{2+\omega}}\tilde{C} \right]^{1/2} dV \tag{A-3}$$

which has no direct solution but can be solved by approximation techniques. We have used the Simpson's Rule(10) with the result

$$\int_{V_c}^{V_c+2h} f(V)dV = \frac{h}{3}\left[f(V_c) + 4f(V_c+h) + f(V_c+2h)\right] \tag{A-4}$$

where $V(u=0) = V_c + 2h$. By letting this limit equal to $1 + \lambda$ we can introduce λ as the fractional increase in the specific volume over unity at the location where the particle velocity is zero. This method of handling the coefficient h reduces the propagation of computational errors and allows a convenient way to enter the fraction part of volume into the iterative program.

Replacing the integrand of Eqn. A-3 with its functional counterpart in Eqn. A-4 and simplifying the resulting expression, we find

$$\frac{5(1-V_c)-\lambda}{1-V_c+\lambda} = 4\left[R_1\tilde{A}e^{-R_1(1+V_c+\lambda)/2} + R_2\tilde{B}e^{-R_2(1+V_c+\lambda)/2} + \frac{(1+\omega)\tilde{C}}{[(1+V_c+\lambda)/2]^{2+\omega}} \right]^{1/2}$$

$$+\left[R_1\tilde{A}e^{-R_1(1+\lambda)} + R_2\tilde{B}e^{-R_2(1+\lambda)} + \frac{(1+\omega)\,\tilde{C}}{(1+\lambda)^{2+\omega}} \right]^{1/2} \qquad \text{(A-5)}$$

Using the available data base(5,6) with reported values of R_1, R_2, V_c, $\tilde{E}_o$, and ω, one can easily determine the value of λ and in turn the value of V(u=0) for each explosive in that data base. These values are listed in Table 1. As one can easily note, the value of V(u=0) for all the explosives listed in that table remains the same within a standard deviation of less than 0.5% from an average value of 1.119. Having established the uniqueness of this value for most of the H-C-N-O explosives, we can use it in Eqn. A-5 to determine the value of R_1 and R_2 for any new explosive. This procedure is somewhat more involved because now each iteration for the principal eigenvalue of R_1 will require reevaluation of all coefficients R_2, $\tilde{A}$, $\tilde{B}$ and $\tilde{C}$; i.e., one has to recalculate all normalized pressure coefficients after each pass through the algorithm.

$$(R_1)_{n+1} = (R_1)_n - F/F' \qquad \text{(A–6)}$$

Here, F symbolizes Eqn. A-5 when the left-hand side of the equation is moved to the right-hand side so that the value of F represents the remainder to be nulled out by the iteration scheme and

$$F' = \partial F/\partial R_1 \qquad \text{(A–7)}$$

This procedure is in effect the steepest prescription for convergence and will yield the full set of eigenvalues and pressure coefficients which are described in the text.

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Figure Captions

Fig. 1 Adiabatic expansion of the reaction products of a generic explosive whose characteristic values are listed in Table 2.

Fig. 2 The effect of $\tilde{E}_0$ on the JWL gamma profile.

Fig. 3 The effect of V(u=0) on the JWL gamma profile.

Fig. 4 The effect of κ and V(u=0) on the JWL gamma profile

a) V(u=0) = 1.119 $\kappa = 0.27 \pm .04$

b) V(u=0) = $1.119 \pm .01$ $\kappa = 0.23$

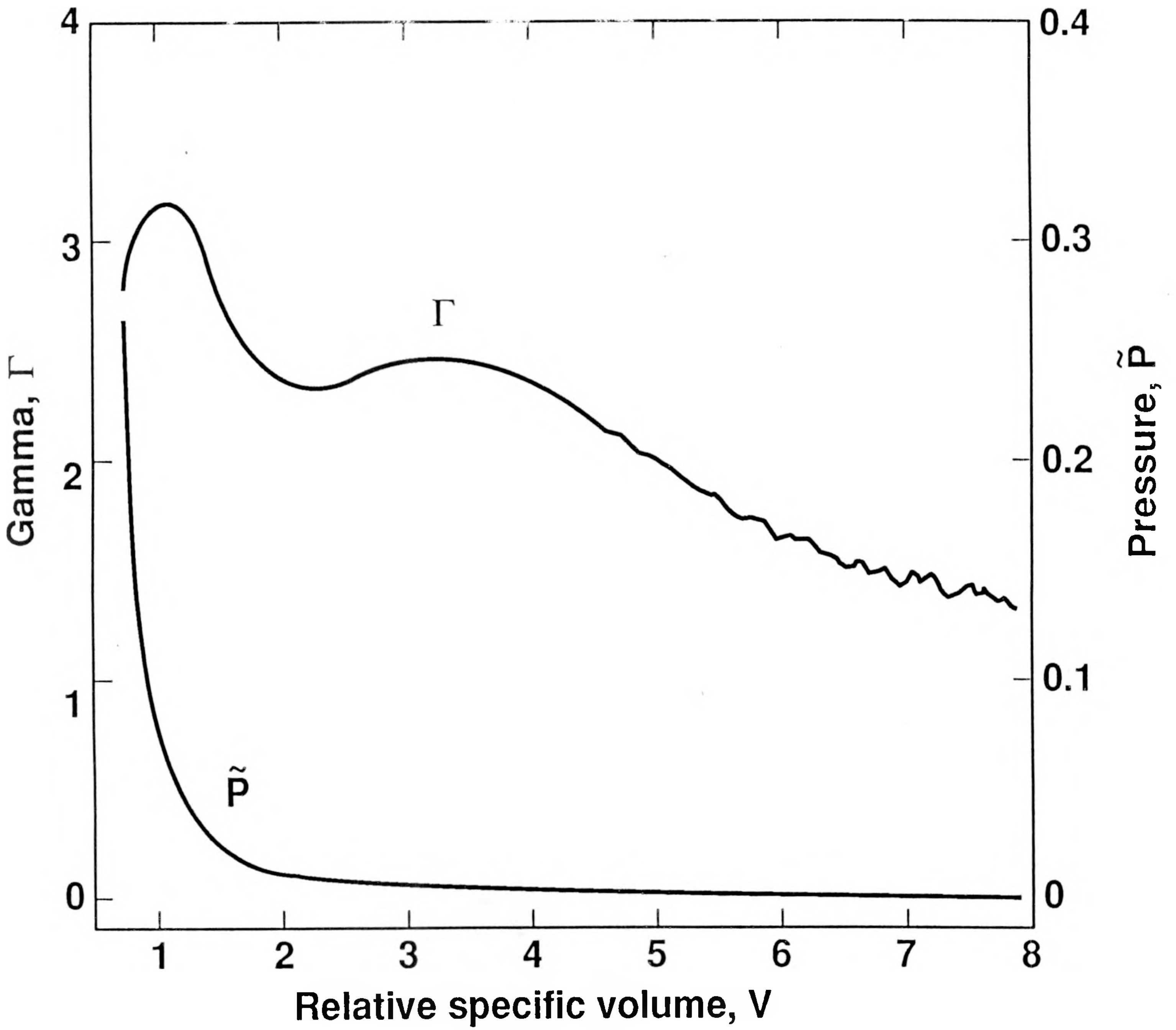

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Fig. 1 Adiabatic expansion of the reaction products of a generic explosive whose characteristic values are listed in Table 2.

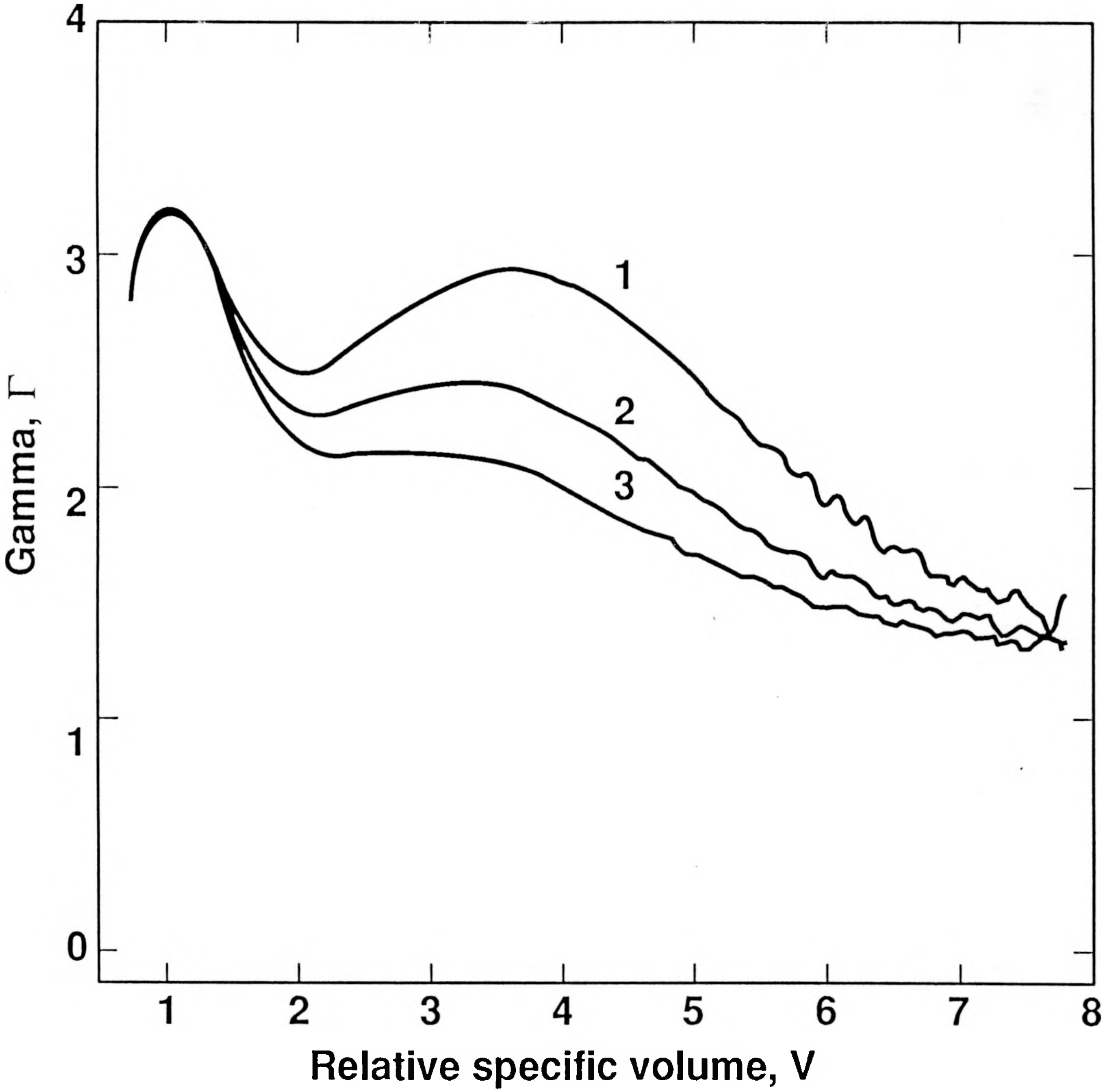

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Fig. 2 The effect of $\tilde{E}_0$ on the JWL gamma profile.

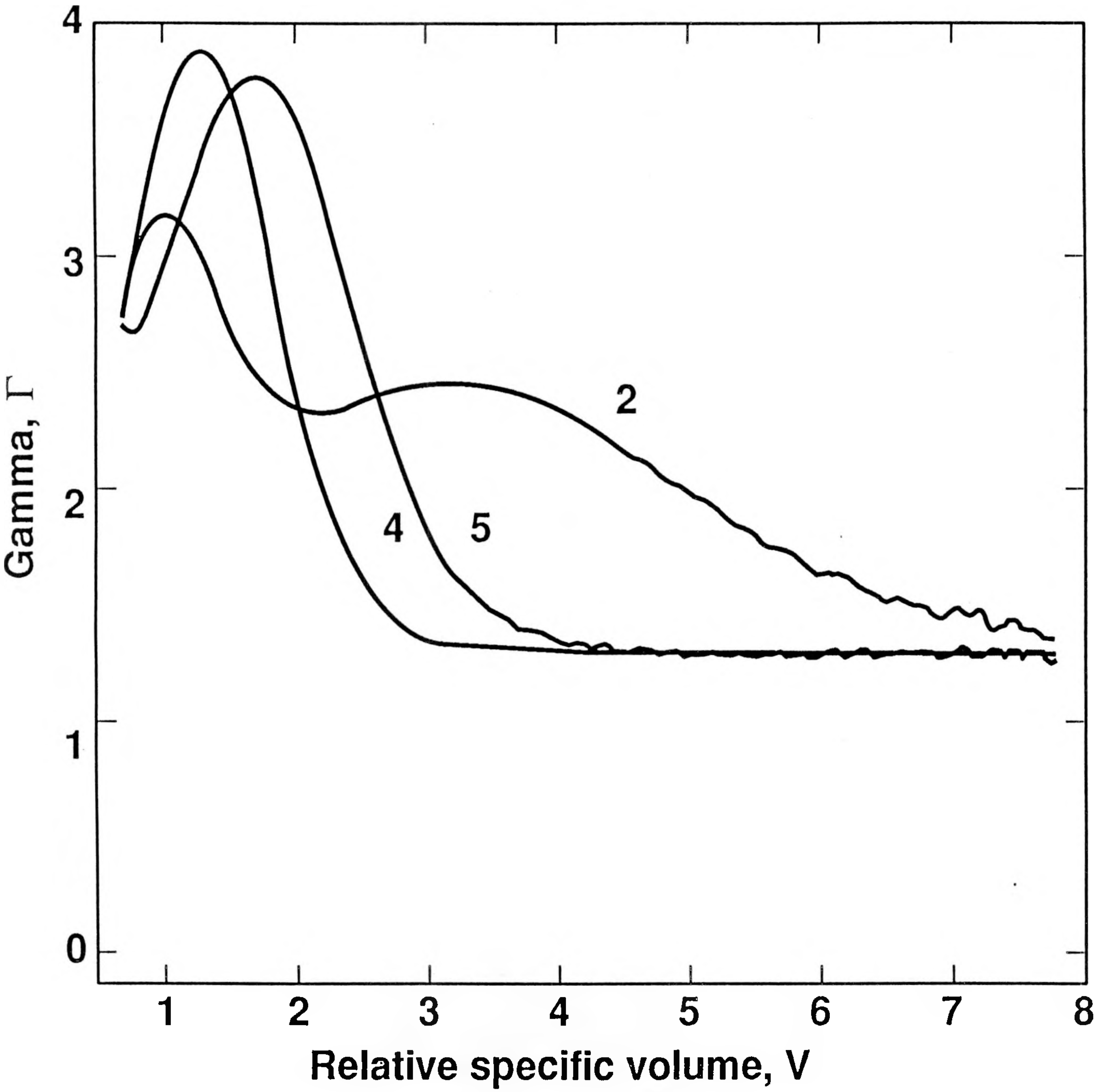

Fig. 3 The effect of V(u=0) on the JWL gamma profile.

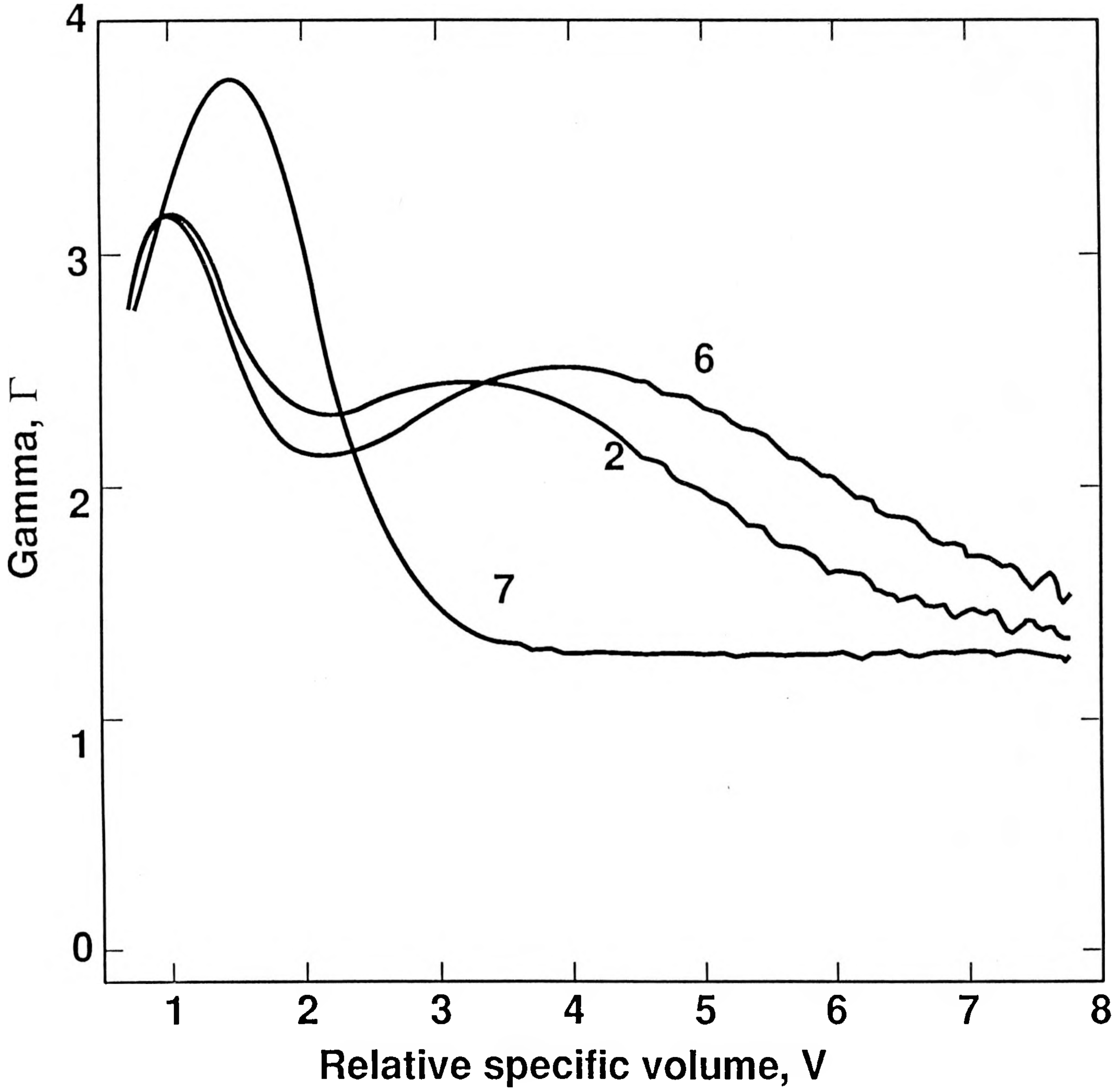

Fig. 4a The effect of κ on the JWL gamma profile.

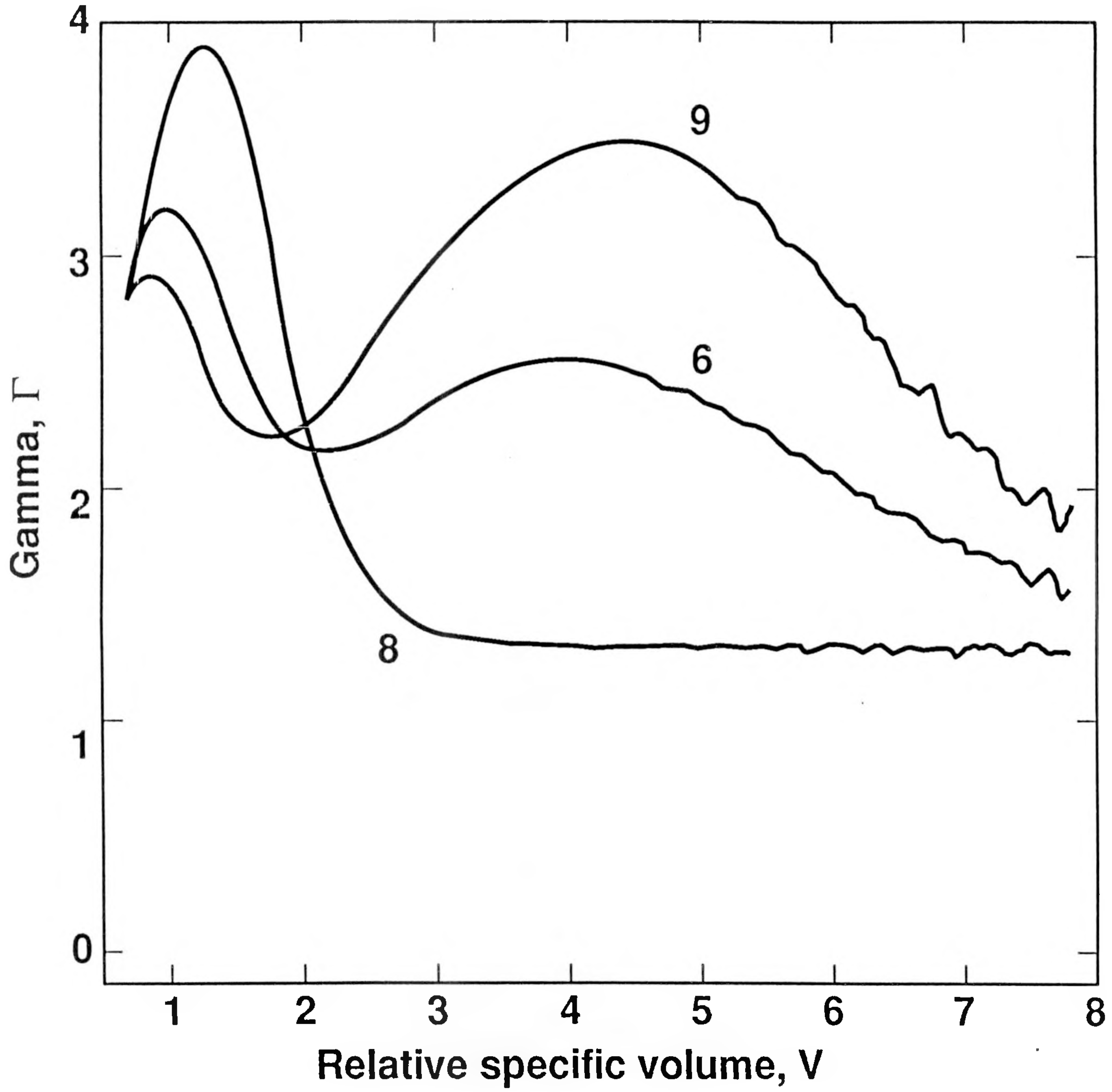

Fig. 4b The effect of V(u=0) with κ = 0.23 on the JWL gamma profile.

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