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Analytical Representation of the Adiabatic Equation for Detonation Products Based on Statistical Mechanics and Intermolecular Forces [and Discussion]

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Analytical representation of the adiabatic equation for detonation products based on statistical mechanics and intermolecular forces

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A new mathematical form is presented for the equation of state of a detonation product fluid along the adiabat describing its expansion from the Chapman–Jouguet state. The basic ansatz is a rational function form for the adiabatic gamma coefficient in terms of the reduced density V_{cj}/V as variable, from which the pressure can be derived analytically, and the internal energy by quadrature. Rational approximants of arbitrary order can be fitted by linear least squares to results from an ideal detonation code involving a fundamental equation of state based on statistical mechanics and intermolecular forces. The approximants can be checked for accuracy, and used in hydrodynamic codes. The method is illustrated by application to results for pentaerythritol tetranitrate, and the new equations are compared with the Jones–Wilkins–Lee equation.

1. Introduction

There are now in existence quite a few sophisticated ideal detonation codes incorporating an equation of state (EOS) for detonation products based on statistical mechanics and intermolecular forces (Chirat & Pittion-Rossillon 1981; Ree 1984; Freeman *et al.* 1991). They are being increasingly used by researchers pursuing fundamental studies in condensed phase detonation. However, to fit experimental detonation results from cylinder and other tests for the expansion adiabat, comparatively simple equations relating the pressure P and the internal energy E (and possibly the temperature T) to the volume V, in which the complex chemistry of the detonation products is implicit, are almost mandatory. The assumption behind such equations is that all the chemical reactions are at equilibrium. A similar but more general reactive adiabatic (non-equilibrium) equation, which contains in addition one or more extent-of-reaction parameters λ, is required to model non-ideal detonation in finite element hydrodynamic codes.

By contrast with the sophisticated and fundamental EOS used in modern detonation codes, the equilibrium and reactive adiabatic equations most commonly used are either empirical (e.g. Jones–Wilkins–Lee (JWL) equation) or simplistic (e.g. polytropic EOS). In addition they are usually inconsistent with the fundamental EOS (e.g. assume constant Gruneisen gamma or constant heat capacity), and are relatively inflexible. There is clearly a need for both reactive and equilibrium (isentropic) adiabatic equations which are consistent with the ideal detonation codes. The easiest way to achieve this goal is to devise appropriate flexible forms for PVE and $PVE\lambda$ equations and to fit them to detonation code results.

The aim of this paper is to propose a particular form for the analytical

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representation of the equilibrium adiabatic expansion results from ideal detonation codes, and to present a procedure for generating approximants of any desired accuracy.

2. Thermodynamics

An equilibrium adiabatic expansion equation is essentially an equation for the pressure P of a fluid mixture as a function of the specific volume V (i.e. volume per unit mass) for constant specific entropy S, since an equilibrium adiabat is also an isentrope; that is,

$$P = P(V) \quad \text{for} \quad S = \text{const.} \tag{2.1}$$

A quantity of great importance in describing ideal detonation and adiabatic expansion is the adiabatic gamma coefficient defined by

$$\Gamma_S = -(\partial \log P/\partial \log V)_S, \tag{2.2}$$

where the derivative is to be taken under the conditions of chemical (and phase) equilibrium, and constant mass of each chemical element present (gibbsian derivative). In view of its experimental and theoretical importance, in many ways the variation of Γ_S with volume V makes a better starting point for developing an adiabatic equation than the pressure P itself. Γ_S varies, often monotonically, from the value γ_{cj} at the Chapman–Jouguet (CJ) state of around 3, to the perfect gas value γ_{id} of around 1.3 at infinite volume.

A more convenient variable in a formal mathematical sense than V or V/V_{cj} is $x = \log(V/V_{\text{cj}})$, which varies from zero at the CJ state to infinity. If the adiabatic gamma is known as a function of x then the pressure P is given by

$$P = P_{\text{cj}} \exp\left[-\int_0^x \Gamma_S(x')\,\mathrm{d}x'\right]. \tag{2.3}$$

The specific internal energy E along the adiabat is also of interest. The fundamental differential equation of thermodynamics for a fixed (unit) mass of a single phase fluid mixture is

$$\mathrm{d}E = T\,\mathrm{d}S - P\,\mathrm{d}V + \sum_{i=1}^{S} \mu_i\,\mathrm{d}n_i, \tag{2.4}$$

where μ_i is the chemical potential and n_i the molar mass of the ith species. However, the condition for chemical equilibrium between all the species present is precisely that the summation term always vanishes, so that the differential equation reduces to

$$\mathrm{d}E = T\,\mathrm{d}S - P\,\mathrm{d}V, \tag{2.5}$$

and it follows that the pressure is given by

$$P = -(\partial E/\partial V)_S. \tag{2.6}$$

Therefore by integration from the CJ state at constant entropy the internal energy change is

$$E - E_{\text{cj}} = -\int_{V_{\text{cj}}}^{V} P\,\mathrm{d}V,$$

or

$$E - E_{\text{cj}} = -(PV)_{\text{cj}} \int_0^x \frac{P}{P_{\text{cj}}} \mathrm{e}^{x'}\,\mathrm{d}x'. \tag{2.7}$$

Thus the internal energy along the adiabat can be related directly to the adiabatic gamma coefficient as a function of x by

$$\frac{E-E_{\mathrm{cj}}}{(PV)_{\mathrm{cj}}} = -\int_0^x \exp\left\{-\int_0^{x'} [\Gamma_S(x'')-1]\,\mathrm{d}x''\right\}\mathrm{d}x'. \tag{2.8}$$

Note that if Γ_S is constant, which is true for a polytropic perfect gas, defined as one for which the heat capacity C_V is a constant, independent of temperature, then we get the simple form familiar to detonation theorists

$$E-E_{\mathrm{cj}} = \frac{PV-(PV)_{\mathrm{cj}}}{(\Gamma_S-1)}, \tag{2.9}$$

where Γ_S is the ratio of the heat capacities C_P/C_V.

Another important thermodynamic quantity occurring in the equations of motion describing detonation is the Gruneisen gamma coefficient defined by

$$\Gamma_{\mathrm{G}} = -(\partial \log T/\partial \log V)_S, \tag{2.10}$$

where, again, the derivative is to be taken under the conditions of chemical and phase equilibrium, and constant mass of each chemical element present. If Γ_{G} is known as a function of $x = \log(V/V_{\mathrm{cj}})$ then the temperature can be derived by integration by analogy with (2.3), namely

$$T = T_{\mathrm{cj}} \exp\left[-\int_0^x \Gamma_{\mathrm{G}}(x')\,\mathrm{d}x'\right]. \tag{2.11}$$

Knowledge of P, T and E as functions of density along the expansion adiabat gives a fairly comprehensive picture of the thermodynamic behaviour of the detonation fluid.

3. Rational representation

This paper is based on the following ansatz for the adiabatic gamma coefficient:

$$\Gamma_S(\rho) = \sum_{j=0}^{N} a_j \rho^j \Big/ \sum_{j=0}^{N} b_j \rho^j, \tag{3.1}$$

that is, the ratio of two polynomials of equal degree $N = 1, 2, 3$, etc., in the reduced density $\rho = V_{\mathrm{cj}}/V$, containing $2N+2$ coefficients. One coefficient, say b_N, is arbitrary and set equal to unity: $b_N = 1$. In addition, for $\rho = 0$ we have $a_0 = \gamma_{\mathrm{id}} b_0$, where γ_{id} is the perfect gas value of Γ_S. The essential dependence of Γ_S on ρ is thus determined by $2N$ coefficients.

Given a set of pairs of values ρ_k, $\gamma_k = \Gamma_S(\rho_k)$ for $k = 1, 2, 3, \ldots, M$ from an ideal detonation code (or experiment), the a and b coefficients can be found by solving the linear equations

$$b_0(\gamma_{\mathrm{id}}-\gamma_k) + \sum_{j=1}^{N-1} (a_j - b_j\gamma_k)\,\rho_k^j + a_N \rho_k^N = \gamma_k \rho_k^N, \tag{3.2}$$

for $k = 1, 2, 3, \ldots, M$, provided $M \geqslant 2N$. If $M > 2N$ then a singular value decomposition technique, which is equivalent to the linear least squares method, can be used to get the best values of the coefficients.

The rational form (3.1) is not mathematically suitable in general for deriving the adiabatic equation proper for the pressure by integration. For this purpose it can be transformed by factorizing the denominator polynomial $B(\rho)$ in (3.1)

$$B(\rho) = \prod_{j=1}^{N} (\rho+\beta_j), \tag{3.3}$$

where the β parameters are the negatives of the roots of $B(\rho)$, that is

$$B(-\beta_j) = 0 \quad (j = 1, 2, \dots, N). \tag{3.4}$$

Then Γ_S can be partial fractioned to

$$\Gamma_S(\rho) = \gamma_{\mathrm{id}} + \rho \sum_{j=1}^{N} \frac{\alpha_j}{\rho+\beta_j}, \tag{3.5}$$

where the αs are as yet unknown. To find the α parameters, substitute for Γ_S from (3.1) into (3.5) to get

$$A(\rho) = \gamma_{\mathrm{id}} B(\rho) + \rho \sum_{i=1}^{N} \alpha_i B_i(\rho), \tag{3.6}$$

where $A(\rho)$ is the numerator polynomial in (3.1) and

$$B_i(\rho) = B(\rho)/(\rho+\beta_i) \quad (i = 1, 2, \dots, N). \tag{3.7}$$

Put $\rho = -\beta_j$ to get

$$A(-\beta_j) = -\beta_j \sum_{i=1}^{N} \alpha_i B_i(-\beta_j). \tag{3.8}$$

Now $B_i(-\beta_j)$ vanishes unless $i = j$, so

$$A(-\beta_j) = -\beta_j \alpha_j B_j(-\beta_j). \tag{3.9}$$

But by differentiating (3.3) the derivative $B'(\rho)$ of $B(\rho)$ can be written

$$B'(\rho) = \sum_{i=1}^{N} B_i(\rho), \tag{3.10}$$

so $B'(-\beta_j) = B_j(-\beta_j)$. Hence

$$\alpha_j = -A(-\beta_j)/\beta_j B'(-\beta_j) \quad (j = 1, 2, \dots, N). \tag{3.11}$$

Note that if the βs are real they must be positive, but they may also be complex, when they occur in conjugate pairs, thus ensuring the reality of Γ_S. By substituting (3.5) into (2.3) we get for the adiabatic pressure equation

$$P = P_{\mathrm{cj}} \rho^{\gamma_{\mathrm{id}}} \prod_{j=1}^{N} \left(\frac{\rho+\beta_j}{1+\beta_j}\right)^{\alpha_j}, \tag{3.12}$$

$$\frac{E-E_{\mathrm{cj}}}{(PV)_{\mathrm{cj}}} = -\int_{\rho}^{1} r^{\gamma_{\mathrm{id}}-2} \prod_{j=1}^{N} \left(\frac{r+\beta_j}{1+\beta_j}\right)^{\alpha_j} \mathrm{d}r. \tag{3.13}$$

For $N = 1$ the integral can be written in terms of the incomplete beta function. In the general case it must be evaluated by numerical integration, but since the integrand is well-behaved everywhere, this can be carried out easily, quickly and accurately using standard algorithms.

The same type of rational approximation can be used for the Gruneisen gamma coefficient, $\varGamma_G$, defined by (2.10), that is

$$\varGamma_G(\rho) = \sum_{j=0}^{N} c_j \rho^j \Big/ \sum_{j=0}^{M} d_j \rho^j. \tag{3.14}$$

The development is exactly the same as for $\varGamma_S$, and leads to

$$\varGamma_G(\rho) = \gamma_{id} - 1 + \rho \sum_{j=1}^{N} \frac{\xi_j}{\rho + \eta_j}, \tag{3.15}$$

since the perfect gas value of $\varGamma_G$ is $\gamma_{id} - 1$, where the η parameters are the negatives of the roots of the denominator $D(\rho)$ of (3.14), and the ξ parameters are given by the analogues of (3.11). This equation can be integrated analytically to yield the following analogue of (3.12) for the temperature along the adiabat:

$$T = T_{cj} \rho^{\gamma_{id}-1} \prod_{j=1}^{N} \left(\frac{\rho + \eta_j}{1 + \eta_j}\right)^{\xi_j}. \tag{3.15}$$

4. Application to PETN

Figure 1 is a plot of the adiabatic gamma coefficient $\varGamma_S$ as a function of the reduced volume V/V_{cj} along the expansion adiabat for the ideal detonation of pentaerythritol tetranitrate (PETN) at an initial density of 1 g cm^{-3}. The points are calculated from the ideal detonation code called IDeX developed for ICI plc (Freeman *et al.* 1991) which is based on an analytical representation of the statistical thermodynamic equation of state for mixtures of molecules interacting with the Buckingham exponential-α:6 potential (Byers Brown 1987; Byers Brown & Horton 1988; Byers Brown & Braithwaite 1989). The solid line is the rational least squares fit to the $M = 50$ points for $N = 2$. The values of the a and b coefficients are given in table 1; note that $\gamma_{id} = a_0/b_0 = 1.220$.

In figure 2 the IDeX results for log (P/P_{cj}) are plotted against V/V_{cj} and compared with equation (3.12) for $N = 2$; that is,

$$P = P_{cj} \rho^{\gamma_{id}} \left(\frac{\rho + \beta_1}{1 + \beta_1}\right)^{\alpha_1} \left(\frac{\rho + \beta_2}{1 + \beta_2}\right)^{\alpha_2}, \tag{4.1}$$

where $\rho = V_{cj}/V$. In this case the coefficients α and β turn out to be complex conjugate pairs, and calculations can be carried out either by using complex arithmetic, or by using the real form

$$\log(P/P_{cj}) = \gamma_{id} \log \rho + \tfrac{1}{2}(a_2 - \gamma_{id}) \log [\mathrm{B}(\rho)/B(1)] + \frac{[2a_1 - b_1(a_2 + \gamma_{id})]}{D}\left[\arctan\left(\frac{2\rho + b_1}{D}\right) - \arctan\left(\frac{2 + b_1}{D}\right)\right], \tag{4.2}$$

where here

$$D = \surd(4b_0 - b_1^2). \tag{4.3}$$

The agreement is again very satisfactory, with a root mean square (RMS) deviation of 4×10^{-4}.

Figure 3 shows a similar graph for the reduced internal energy quantity of §2, calculated from (3.13) by the alternative extended Simpson's rule. In this case the

Figure 1

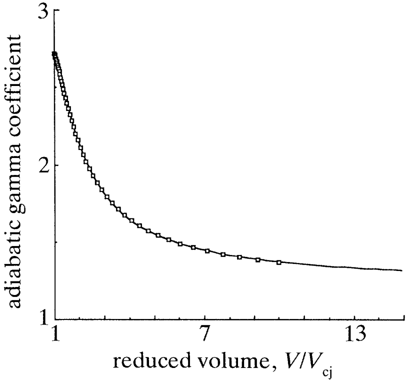

Figure 2

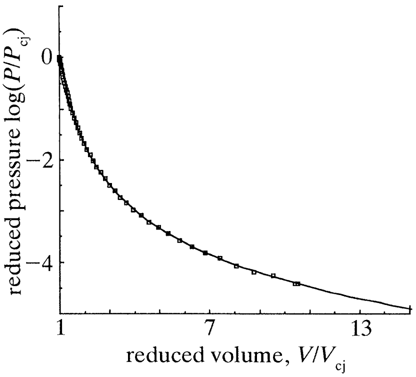

Figure 3

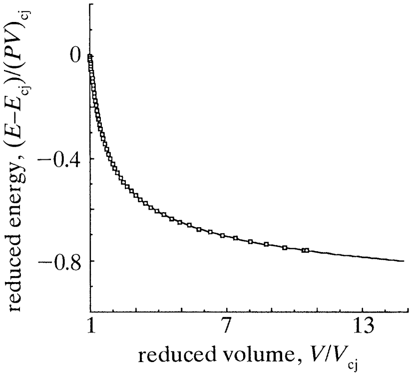

Figure 4

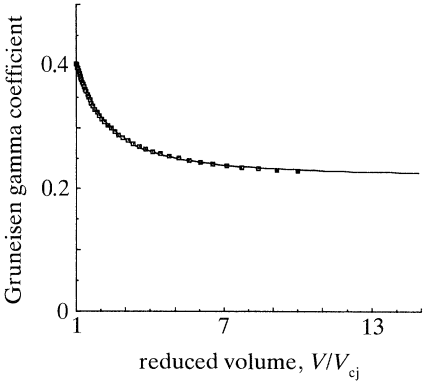

Figure 1. The adiabatic gamma coefficient for PETN (initial density 1 g cm^{-3}) as a function of volume along the expansion adiabat. Squares are calculated from an ideal detonation code. The line is the rational fit of order 2.

Figure 2. Log of the reduced pressure P/P_{cj} for PETN (initial density 1 g cm^{-3}) as a function of volume. Squares are calculated from an ideal detonation code. The line is derived from the rational fit of order 2.

Figure 3. A reduced internal energy for PETN (initial density 1 g cm^{-3}) as a function of volume. Squares are calculated from an ideal detonation code. The line is derived from the rational fit of order 2.

Figure 4. The Gruneisen gamma coefficient for PETN (initial density 1 g cm^{-3}) as a function of volume along the expansion adiabat. Squares are calculated from an ideal detonation code. The line is the rational fit of order 2.

Table 1. *Coefficients in numerator and denominator of equation (3.1) for the adiabatic gamma coefficient* Γ_S *for the expansion of the detonation products of PETN at an initial density of 1.00* g cm^{-3}, *as determined by a linear least square criterion*

i	a_i	b_i
0	1.1741	0.9624
1	0.7493	−0.4702
2	2.1383	1

Table 2. *Coefficients in numerator and denominator of equation (3.14) for the Gruneisen gamma coefficient* Γ_G *for the expansion of the detonation products of PETN at an initial density of 1.00* g cm^{-3}, *as determined by a linear least square criterion*

i	c_i	d_i
0	0.1084	0.4928
1	0.3027	1.2747
2	0.7105	1

RMS deviation is even smaller, 3×10^{-5}, which is only to be expected since the original fitting is to a higher derivative.

Figure 4 is a plot of the Gruneisen gamma coefficient Γ_G as a function of the reduced volume V/V_{cj} along the expansion adiabat for the ideal detonation of PETN at an initial density of 1 g cm^{-3}. The points are again calculated from the IDeX ideal detonation code, and the solid line is the rational approximation for $N = 2$, with coefficients given in table 2, and a RMS deviation of 0.004. The temperature T along the adiabat can then be calculated from (3.15), and a plot of the result looks very similar to figure 2 for the pressure, and will therefore not be presented. The RMS deviation for the fit with $N = 2$ is 2×10^{-4}.

5. Comparison with other adiabatic equations

The two adiabatic equations in common use are the very simple polytropic (perfect gas) equation mentioned in §2, and the JWL equation (Lee *et al.* 1968), which has the form

$$P = (K/V^{\gamma_{id}}) + P_1 e^{-V/V_1} + P_2 e^{-V/V_2}, \tag{5.1}$$

and contains five constants in addition to γ_{id}. The first term is that for a perfect gas, and the two exponential terms, which dominate near the CJ state, describe departures from ideal behaviour. The integrated form of the JWL equation (Lee *et al.* 1968) implies that the Gruneisen gamma coefficient Γ_G is a constant equal to $\gamma_{id} - 1$, which as can be seen from figure 4 is a poor approximation.

The JWL equation has received recent support from Cooper (1989), who has suggested from empirical evidence a two-piece common reduced form for the pressure as a function of particle velocity, which Lambourn (1989) has shown implies an adiabatic equation very similar to the JWL but with only one exponential term.

For comparison, the rational form for Γ_S with $N = 2$ leads to the pressure equation (3.12) which may be written

$$P = \frac{K}{V^{\gamma_{id}}}\left(1 + \frac{V_1}{V}\right)^{\alpha_1}\left(1 + \frac{V_2}{V}\right)^{\alpha_2}. \tag{5.2}$$

Both (5.1) and (5.2) have four parameters in their reduced forms, but the striking advantage of (5.2) is that the parameters can be obtained by linear algebra from calculated or experimental values of the adiabatic gamma coefficient Γ_S. By contrast, the JWL expression for Γ_S is complicated and involves the parameters nonlinearly. This gives rise to the difficulty that solutions for the parameters are not unique, and may only correspond to local minima. Fits easily lead to double maxima in Γ_S of doubtful physical significance, which have been much discussed, but certainly do not occur in the adiabats of single substances. If a satisfactory fit cannot be obtained with four parameters, (5.2) is easily extended to a larger number, which can be easily calculated. By contrast, the extension of (5.1) gravely increases the difficulty of finding the best parameters.

A thermodynamic argument in favour of (5.2) and against (5.1) is that for a slightly imperfect gas, whose deviations from perfect behaviour can be adequately described by including the second virial coefficient $B(T)$ in the equation of state, the adiabatic gamma has the form

$$\Gamma_S = \gamma_{\text{id}} + \rho[\gamma B + 2\gamma(\gamma-1)\,TB' + (\gamma-1)^2T^2B''] + O(\rho^2), \tag{5.3}$$

where the primes denote differentiation with respect to T and $\gamma = \gamma_{\text{id}}$. Since T is roughly proportional to $\rho^{\gamma-1}$ along the adiabat, and $B(T)$ can be expanded as a power series in $1/T$ beginning with a constant, Γ_S begins with a term linear in ρ. Now (3.1) or (3.5) can clearly be expanded in powers of the density ρ, but the corresponding expression for the JWL equation has essential singularities as a function of ρ at $\rho = 0$, and can not be so expanded. It is therefore inconsistent with the well established virial expansion of statistical mechanics.

6. Conclusions

A simpler, accurate rational alternative to the JWL equation for describing the adiabatic expansion of detonation fluid has been presented. It is particularly suitable for fitting to the calculated results from ideal detonation codes for use in hydrodynamic computations. When phase changes occur causing discontinuities in derivatives, it should be possible to use matched piece-wise fits, and the method should also be capable of extrapolation to the vicinity of a given adiabat and to the supracompression region.

The next major step is to generalize the equation to cover reactive adiabats by introducing an extent of reaction parameter λ.

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References

Byers Brown, W. 1987 Analytical representation of the excess thermodynamic equation of state for classical fluid mixtures of molecules interacting with α-exponential-6 pair potentials up to high densities. *J. chem. Phys.* **87**, 566–577.

Byers Brown, W. & Braithwaite, M. 1989 Sensitivities of adiabatic and Gruneisen gammas to errors in molecular properties of detonation products. In *Proc. Ninth Symp. (Int.) on Detonation*, pp. 271–283. Naval Surface Weapons Center, Whiteoak, Maryland, U.S.A.

Byers Brown, W. & Horton, T. V. 1988 Analytical representation of high density fluid equations of state based on statistical mechanics. In *Shock waves in condensed matter 1987* (ed. S. C. Schmidt & N. C. Holmes), pp. 77–80. The Netherlands: Elsevier Science.

Chirat, R. & Pittion-Rossillon, G. 1981 Detonation properties of condensed explosives calculated with an equation of state based on intermolecular potentials. In *Proc. Seventh Symp. (Int.) on Detonation*, pp. 703. Naval Surface Weapons Center, Whiteoak, Maryland, U.S.A.

Cooper, P. W. 1989 Shock behaviour of explosives about the CJ point. In *Proc. Ninth Symp. (Int.) on Detonation*, pp. 379–385. Naval Surface Weapons Center, Whiteoak, Maryland, U.S.A.

Freeman, T. L., Gladwell, I., Braithwaite, M., Byers Brown, W., Lynch, P. M. & Parker, I. B. 1991 Modular software for modelling the ideal detonation of explosives. *Math. Engng Ind.* **3**, 97–109.

Lambourn, B. D. 1989 In *Proc. Ninth Symp. (Int.) on Detonation*, pp. 385–386. Naval Surface Weapons Center, Whiteoak, Maryland, U.S.A.

Lee, E. L., Hornig, H. C. & Kury, J. W. 1968 Adiabatic expansion of high explosive detonation products. Lawrence Radiation Laboratory, *Rep. No. UCRL-50422*.

Ree, F. H. 1984 *J. chem. Phys.* **71**, 1251.

Discussion

B. D. Lambourn (*AWE, Aldermaston, U.K.*). (*a*) I believe the JWL equation of state adiabatic gamma does have acceptable behaviour as volume tends to infinity; in fact $\Gamma_S \rightarrow 1+\omega$. (*b*) All the experimental data from the U.K., U.S.A. and France shows that when detonation products are expanded into compressed gases from a one-dimensional detonation wave, the CJ adiabat dips below the constant Γ_S adiabat, implying that $\mathrm{d}\Gamma_S/\mathrm{d}v|_{V=V_{\mathrm{cj}}} > 0$. This behaviour is matched by a JWL double exponential form or a single exponential form for the pressure-volume relation along the adiabat, but not by the THEOSTAR/IDeX predictions.

W. Byers Brown. (*a*) As I show in my paper, although the adiabatic gamma coefficient, Γ_S, for the JWL equation goes to the correct limit γ_{id} ($1 = \omega$ in the usual notation) it does not approach this value in the way required by statistical thermodynamics. The virial expansion requires that (in my notation)

$$\lim_{V<\infty}\,(\Gamma_S-\gamma_{\mathrm{id}})V \text{ is non-zero,}$$

where the value involves the second virial coefficient, as shown in equation (5.3) of the text. On the other hand, the JWL equation predicts that this limit vanishes, and indeed that

$$\lim_{V\rightarrow\infty}\,(\Gamma_S-\gamma_{\mathrm{id}})\,V^n = 0 \quad (\text{all } n).$$

(*b*) The concern is because the plot of Γ_S against volume in figure 1, calculated from the IDeX ideal detonation code based on my THEOSTAR equation of state (Byers Brown 1987), does not exhibit a maximum. However, as stated, this plot is for PETN at a loading density of 1.00 g cm^{-3}. At the maximum loading density of 1.77 g cm^{-3} the corresponding plot does indeed exhibit a maximum, but it also exhibits a discontinuity in slope due to the solid carbon in the detonation products. I did not want to use this more complicated case to illustrate the rational approximant for Γ_S, because it requires a two-piece fit. However, there is no problem in principle or practice in constructing such a fit.