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JWL EQUATION OF STATE

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Abstract

The JWL equation of state (EOS) is frequently used for the products (and sometimes reactants) of a high explosive (HE). Here we review and systematically derive important properties. The JWL EOS is of the Mie-Grüneisen form with a constant Grüneisen coefficient and a constant specific heat. It is thermodynamically consistent to specify the temperature at a reference state. However, increasing the reference state temperature restricts the EOS domain in the (V, e) -plane of phase space. The restrictions are due to the conditions that $P \geq 0$, $T \geq 0$, and the isothermal bulk modulus is positive. Typically, this limits the low temperature regime in expansion. The domain restrictions can result in the P - T equilibrium EOS of a partly burned HE failing to have a solution in some cases. For application to HE, the heat of detonation is discussed. Example JWL parameters for an HE, both products and reactions, are used to illustrate the restrictions on the domain of the EOS.

Functional form for JWL pressure

The pressure for the Jones-Wilkins-Lee (JWL) equation of state (EOS) is defined by [Kury *et al.*, 1965; Lee *et al.*, 1968]

$$P(V, e) = A \left[1 - \frac{\omega V_0}{V R_1} \right] \exp(-R_1 V/V_0) + B \left[1 - \frac{\omega V_0}{V R_2} \right] \exp(-R_2 V/V_0) + \frac{\omega}{V} (e + \Delta e) , \quad (1)$$

where $\rho_0 = 1/V_0$ is the initial density, ω is the Grüneisen coefficient $V(\partial_e P)_V$, and A , B , R_1 , R_2 are parameters. The parameters A and B have dimensions of pressure, while R_1 , R_2 and ω are dimensionless. They are subject to the constraints that $R_1 > R_2 > 0$ and $\omega > 0$. Moreover, for explosive products $A > B > 0$. But when used for reactants $A > -B > 0$.

Δe is an offset in the origin of specific internal energy. For the reactants of an explosive, Δe can be chosen such that for the ambient state specified by (V_0, P_0, T_0) , the specific energy $e_0 = 0$. For the products, Δe corresponds to the heat of detonation when the initial state of the reactants is such that $e_0 = 0$ and $P_0 = 0$. This will be shown in a later section.

Isentropes

For HE products, the isentrope through the CJ state is important for applications and simulations. Isentropes also play an important role in constructing the thermal component for the JWL EOS. They are determined by the integral curves of the ODE

$$de/dV = -P(V, e) . \quad (2)$$

It can easily be verified that the isentropes are given by

$$P_C(V) = A \exp(-R_1 v) + B \exp(-R_2 v) + C v^{-\omega-1} , \quad (3a)$$

$$e_C(V) = -\Delta e + V_0 \left[(A/R_1) \exp(-R_1 v) + (B/R_2) \exp(-R_2 v) + (C/\omega) v^{-\omega} \right] , \quad (3b)$$

where $v = V/V_0$ and C is an integration constant with dimensions of pressure that serves to label an isentrope. Later, when the thermal component of the EOS is discussed, the label C will be related to the value of the entropy.

We note the following properties. For all isentropes, $P_C(V) \rightarrow 0$ as $V \rightarrow \infty$. For explosive products, if $C \geq 0$ then $P_C(V) > 0$ for all $V > 0$ and $P_C(V) \rightarrow \infty$ as $V \rightarrow 0$. When $C < 0$, P_C is negative for sufficiently large V .

The isentrope through a state (V_r, e_r) corresponds to

$$C_r = \left[(e_r + \Delta e)/V_0 - (A/R_1) \exp(-R_1 v_r) - (B/R_2) \exp(-R_2 v_r) \right] \omega v_r^\omega, \quad (4)$$

where $v_r = V_r/V_0$. The isentrope can then be used to obtain the sound speed

$$\begin{aligned} c^2(V_r, e_r) &= -V_r^2 (dP_{C_r}/dV)(V_r) = -V_0 v_r^2 (dP_{C_r}/dv)(v_r) \\ &= V_0 \left\{ v_r^2 \left[A R_1 \exp(-R_1 v_r) + B R_2 \exp(-R_2 v_r) \right] + (\omega + 1) \frac{C_r}{v_r^\omega} \right\}. \end{aligned} \quad (5)$$

If $A, B, C_r > 0$, then the isentropic bulk modulus, $K = \rho c^2$, is positive for all $V > 0$. Moreover, $c \rightarrow 0$ as $V \rightarrow \infty$. Later issues that arise when $C_r < 0$ will be discussed.

For any isentrope, the JWL equation of state has the Mie-Grüneisen form,

$$P(V, e) = P_C(V) + \frac{\omega}{V} \left[e - e_C(V) \right]. \quad (6)$$

Equation (1) is identical to Eq. (6) with $C = 0$.

Typically, for explosive products, the JWL parameters are fit to data for the release isentrope from the detonation state. When used for explosive reactants, the parameters are fit to data for the shock locus through the initial state (V_0, e_0) .

Formulation of temperature

To obtain a complete EOS from the JWL pressure, Eq. (1), a thermodynamic consistent temperature needs to be specified. Utilizing the thermodynamic relation

$$(\partial_V T)_S = -(T/V) \omega, \quad (7)$$

and assuming a constant specific heat, \mathcal{C}_V , the JWL temperature can be defined as follows:

1. Select the temperature at a reference point; T_r at (V_r, e_r) .
For products EOS, it is natural to use the CJ state as the reference point. For reactants or inert, it is natural to chose the ambient state (atmospheric pressure and room temperature) as the reference point.
2. The reference isentrope is given by Eqs. (3a) and (3b) with the parameter C_r given by Eq. (4).
3. Along the reference isentrope, the temperature is determined by Eq. (7). Since the Grüneisen coefficient, ω , is constant,

$$T_{C_r}(V) = \left(\frac{V_r}{V}\right)^\omega T_r . \quad (8a)$$

Equation (7) implies that the temperature on all isotherms have this form. Hence, the $T = 0$ isotherm is also an isentrope.

4. For a constant specific heat, the temperature off the reference isentrope is given by

$$T(V, e) = T_{C_r}(V) + \frac{e - e_{C_r}(V)}{\mathcal{C}_V} , \quad (8b)$$

where $e_{C_r}(V)$ is given by Eqs. (3b) and (4).

5. The entropy can then be defined by

$$S(V, e) = \mathcal{C}_V \left[\ln(T(V, e)/T_r) + \omega \ln(V/V_r) \right] + S_r , \quad (9)$$

where S_r is the entropy at the reference state (V_r, e_r) .

Equations (8) and (9) can be combined to give

$$e(V, S) = e_{C_r}(V) + \mathcal{C}_V T_{C_r}(V) \left(\exp \left[\frac{S - S_r}{\mathcal{C}_V} \right] - 1 \right) . \quad (10)$$

This satisfies the fundamental thermodynamic relation

$$de = -P dV + T dS . \quad (11)$$

Since $e(V, S)$ is a thermodynamic potential, Eq. (10) determines a thermodynamically consistent complete EOS. Equations (1), (8) and (9) define the complete JWL EOS with (V, e) as independent thermodynamic variables.

The isentrope label C in Eq. (3) can be mapped into the entropy by substituting Eq. (3b) into Eq. (9);

$$S(C) = S(V, e_C(V)) . \quad (12)$$

The right hand side of Eq. (12) is independent of V since Eq. (2) is consistent with Eq. (11). Moreover, $S(C)$ is a monotonic function; *i.e.*, 1-to-1 map for $C \geq C_0$, where C_0 corresponds to the $T = 0$ isentrope. The function $S(C)$ depends on the choice of the reference temperature T_r . The reference temperature also affects the domain of the EOS. The domain will be discussed in a later section.

We note that $S \rightarrow -\infty$ as $T \rightarrow 0$. Physically, S should go to 0 at $T = 0$. This requires $\mathcal{C}_V \rightarrow 0$ as $T \rightarrow 0$, which is contrary to the assumption of a constant specific heat. The JWL EOS is not meant for low temperature. For a more general derivation of a complete Mie-Grüneisen EOS with a non-constant specific heat see [Menikoff; 2012].

Simplified form

Combining Eqs. (8b), (4), (3a) and (3b), the temperature can be expressed as

$$\mathcal{C}_V T(V, e) = e + \Delta e - V_0 \left[\frac{A}{R_1} \exp(-R_1 v) + \frac{B}{R_2} \exp(-R_2 v) \right] + \frac{\tilde{E}_r}{v^\omega} , \quad (13a)$$

$$\tilde{E}_r = v_r^\omega \left(\mathcal{C}_V T_r - e_r - \Delta e + V_0 \left[\frac{A}{R_1} \exp(-R_1 v_r) + \frac{B}{R_2} \exp(-R_2 v_r) \right] \right) . \quad (13b)$$

Then using Eq. (1) to eliminate $e + \Delta e$, the pressure can be expressed as

$$P(V, T) = A \exp(-R_1 v) + B \exp(-R_2 v) + \omega \left[\frac{\mathcal{C}_V T}{V} - \frac{\tilde{E}_r/V_0}{v^{\omega+1}} \right] . \quad (14)$$

Both $T(V, e)$ and $P(V, T)$ depend on the choice of reference temperature.

If the reference temperature is chosen such that $\tilde{E}_r = 0$,

$$\mathcal{C}_V T_r = e_r + \Delta e - V_0 \left[\frac{A}{R_1} \exp(-R_1 v_r) + \frac{B}{R_2} \exp(-R_2 v_r) \right] , \quad (15)$$

then the expressions for the temperature and pressure simplify

$$\mathcal{C}_V T(V, e) = e + \Delta e - V_0 \left[\frac{A}{R_1} \exp(-R_1 v) + \frac{B}{R_2} \exp(-R_2 v) \right], \quad (16a)$$

$$P(V, T) = A \exp(-R_1 v) + B \exp(-R_2 v) + \frac{\omega}{V} \mathcal{C}_V T. \quad (16b)$$

In this case, for large $V \gg V_0$, the temperature and pressure reduce to

$$\begin{aligned} \mathcal{C}_V T(V, e) &= e + \Delta e, \\ P(V, T) &= \frac{\omega}{V} \mathcal{C}_V T, \end{aligned}$$

and the JWL equation of state limits to an ideal gas equation of state.

Equations (8b), (3b) and (16a) imply that $T = 0$ on the $C = 0$ isentrope. In particular, at V_0 the temperature is zero at $P = A \exp(-R_1) + B \exp(-R_2)$. This can be unrealistically high for detonation products. It is partly due to violating the thermodynamic condition that $\mathcal{C}_V \rightarrow 0$ as $T \rightarrow 0$.

For the EOS of explosive products, $A, B > 0$. A feature of the simplified form of the JWL EOS, Eq. (16), is that the pressure is positive for all $T \geq 0$. In fact, the domain of the EOS is the entire quadrant $T \geq 0$ and $P \geq 0$. Whereas in the (V, e) -plane, the domain is the region above the $C_0 = 0$ isentrope; *i.e.*, $e_{C_0}(V) \geq 0$.

When used for explosive reactants, $A > 0$ and $B < 0$. Then even for $C \geq 0$, the pressure on an isentrope goes negative for sufficiently large V . This restricts the domain of the EOS in the low temperature expansion region.

Domain of EOS

The domain of an EOS is limited by the conditions $T \geq 0$ and $P \geq 0$. From Eq. (3) and Eq. (8b), the isentrope parameters for the reference temperature C_r and for the $T = 0$ isentrope C_0 are related by

$$\begin{aligned} \mathcal{C}_V T_r &= e_{C_r}(V_r) - e_{C_0}(V_r) \\ &= \frac{C_r - C_0}{\omega v_r^\omega}. \end{aligned}$$

The reference state (V_r, e_r) determines C_r . Increasing T_r requires decreasing C_0 . If T_r is larger than the value in Eq. (15) then $C_0 < 0$, and from Eq. (13b), $\tilde{E}_r > 0$. For isentropes with $C < 0$, it follows from Eq. (3a) that the pressure is negative for sufficiently large V . Thus, raising the reference temperature can restrict the low temperature isotherms in expansion.

The domain of an EOS is also limited by thermodynamic stability, which requires that the bulk modulus to be positive. From Eq. (14), the isothermal bulk modulus is

$$\begin{aligned} K_T(V, T) &= -V \left(\frac{\partial P}{\partial V} \right)_T \\ &= v [AR_1 \exp(-R_1 v) + BR_2 \exp(-R_2 v)] + \omega C_V T / V \\ &\quad - \omega(\omega + 1) v^{-\omega-2} \tilde{E}_r / V_0 . \end{aligned} \quad (17)$$

As the temperature of the reference state is raised, \tilde{E}_r increases. For sufficiently large T_r , $\tilde{E}_r > 0$. Then at sufficiently low temperature, even with $A, B > 0$, K_T becomes negative in a portion of the expansion region.

Domain limits may have consequences for simulations. For example, P - T equilibrium of a partly burned explosive will fail to have a solution outside the EOS domain. This can occur in a hydro simulation when a detonation wave hits a free surface and the hot partly burn explosive in the reaction zone expands beyond the initial explosive density.

Heat of detonation

Detonation waves are typically modeled with a single step irreversible reaction; reactants \rightarrow products. The heat of detonation is defined as the change in the heats of formation at standard pressure and temperature, $(P_0, T_0) = (1 \text{ bar}, 25 \text{ C})$;

$$\Delta H_{det} = \Delta H_{prod} - \Delta H_{react} . \quad (18)$$

Since the reaction preserves stoichiometry, this can be re-expressed in terms of the enthalpy ($H = e + P V$) of reactants and products;

$$\Delta H_{det} = H_{prod}(P_0, T_0) - H_{react}(P_0, T_0) . \quad (19)$$

For a high explosive, the initial pressure and temperature are small compared to the values behind the detonation front; *i.e.*, CJ state. To a good approximation, one can take $P_0 = 0$ and $T_0 = 0$. We use this approximation to derive a simple expression for ΔH_{det} .

For the reactants, the initial enthalpy reduces to $H_{react}(P_0, T_0) = e_0$ where $e_0 = e_{react}(P_0, T_0)$. For the products, the JWL EOS goes to an ideal gas in the limit of low density; *i.e.*, from Eq. (14), $V P(V, T) \rightarrow \omega C_v T$ as $V \rightarrow \infty$. Hence, the limit $V \rightarrow \infty$ gives $P = 0$. From Eq. (13), $e(V, T) \rightarrow C_v T - \Delta e$ as $V \rightarrow \infty$. Consequently, $H_{prod}(P_0, T_0) = -\Delta e$. The heat of detonation is then given by

$$\Delta H_{det} = -\Delta e - e_0 . \quad (20)$$

Typically, the energy origin of the reactant EOS is chosen such that $e_0 = 0$. In this case, $\Delta H_{det} = -\Delta e$. For an exothermic reaction, Δe is the heat release.

It is instructive to develop a geometric interpretation for ΔH_{det} . Equation (19) can be re-expressed as

$$\Delta H_{det} = [H_{prod}(V_{cj}, P_{cj}) - H_{react}(V_0, P_0)] - [H_{prod}(V_{cj}, P_{cj}) - H_{prod}(S_{cj}, P_0)] . \quad (21)$$

We note that Eq. (8a) implies the temperature on all isentropes goes to 0 as $V \rightarrow \infty$ or equivalently $P \rightarrow 0$. Hence, $H_{prod}(S_{cj}, P_0) = H_{prod}(P_0, T_0)$. (More generally, $H_{prod}(S_{cj}, P_0) - H_{prod}(P_0, T_0) = [T(S_{cj}, P_0) - T_0] \mathcal{C}_P$, where \mathcal{C}_P is the specific heat at constant pressure.) The Hugoniot jump condition can be express in terms of enthalpy. For a detonation wave,

$$H_{prod}(V_{cj}, P_{cj}) - H_{react}(V_0, P_0) = \frac{1}{2}(V_0 + V_{cj})(P_{cj} - P_0) . \quad (22)$$

Since $(\partial_P H)_S = V$, the change in enthalpy along the CJ release isentrope is

$$H_{prod}(V_{cj}, P_{cj}) - H_{prod}(S_{cj}, P_0) = \int_{P_0}^{P_{cj}} dP V(P, S_{cj}) . \quad (23)$$

Therefore

$$\Delta H_{det} = \frac{1}{2}(V_0 + V_{cj})(P_{cj} - P_0) - \int_{P_0}^{P_{cj}} dP V(P, S_{cj}) . \quad (24)$$

In the (V, P) -plane, the first term corresponds to the area between the P -axis and the segment of the Rayleigh line from P_0 to P_{cj} . Similarly, the second

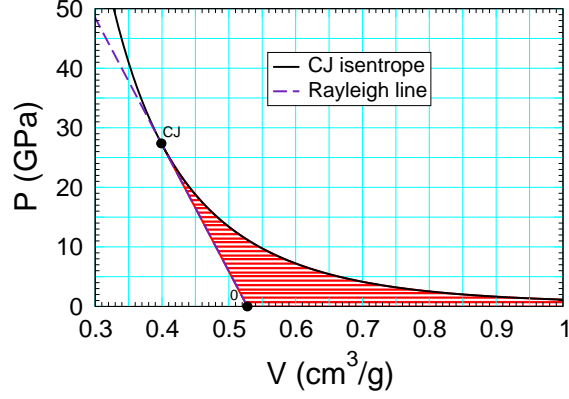


Figure 1: Shaded red area in (V, P) -plane between the CJ release isentrope and the Rayleigh line corresponds to heat of detonation when the release isentrope is extended to $P = 0$ as $V \rightarrow \infty$.

term corresponds to the area between the P -axis and the portion of the release isentrope between P_0 and P_{cj} . Thus, ΔH_{det} corresponds to the area between the Rayleigh line and the CJ isentrope; as shown in figure 1.

To get the full heat of detonation out of an explosive, the product have to expand to a very low pressure and hence a very large specific volume. In practical applications, the volume of expansion is limited. As a rule of thumb V_{final}/V_0 is 7 to 10. For a high explosive this corresponds to $P_{final} \sim 0.1$ GPa. This may be substituted in Eq. (24) to obtain the effective enthalpy that can be extracted from an explosive. It is also worth noting that the data available to calibrate a products EOS extends down to about the same pressure. Thus the full ΔH_{det} depends on extrapolating the EOS, which is likely to introduce a significant error.

Illustrative examples of domain limitations

To illustrate some of the domain issues, we use the JWL parameters calibrated to PBX 9502 in table 1. For the reactants, the choice of Δe shifts the energy origin to give the ambient state, $P_0 = 0$ and $T_0 = 298.15$ K (25 C), with $e_0 = 0$ and the simplified EOS form of Eq. (16). For the products, Δe corresponds to the heat of detonation and is often denoted E_{det} .

Table 1: JWL parameters for PBX 9502 [Tarver & McGuire, 2002, table 1].

	products	reactants	units
A	1361.77	6.3207×10^4	GPa
B	71.99	-4.472	GPa
R_1	6.2	11.3	-
R_2	2.2	1.13	-
ω	0.5	0.8938	-
ρ_0	1.895	1.895	g/cc
V_0	$1/\rho_0 = 0.5277$	$1/\rho_0 = 0.5277$	cc/g
e_0	0.0	0.0	MJ/kg
Δe	$6.9 * V_0$	-0.246929	MJ/kg
C_v	$1.0 \times 10^{-3} * V_0$	$2.487 \times 10^{-3} * V_0$	MJ/(kg·K)

Table 2: CJ detonation state for JWL products EOS of PBX 9502.

V	0.3967	cc/g
ρ	2.5206	g/cc
e	1.8336	MJ/kg
P	28.0	GPa
D	7.716	km/s

The CJ detonation state is determined by the initial state of the reactants (V_0, e_0) , the EOS of the products, and two conditions:

1. The state lies on the detonation locus;

$$e_{\text{cj}} = e_0 + \frac{1}{2}[P(V_{\text{cj}}, e_{\text{cj}}) + P_0] \cdot (V_0 - V_{\text{cj}}) . \quad (25)$$

2. The sonic condition;

$$\frac{P(V_{\text{cj}}, e_{\text{cj}}) - P_0}{V_0 - V_{\text{cj}}} = (\rho c)^2(V_{\text{cj}}, e_{\text{cj}}) . \quad (26)$$

The CJ state is given in table 2. The isentrope, Eq. (3), through the CJ state corresponds to the parameter $C = 0.884$ GPa. The CJ isentrope in

the (V, P) -plane is shown in figure 2. Also shown is the CJ isentrope for a heat of detonation 50 per cent higher. In general, the CJ pressure and the detonation speed increase with increasing Δe .

With the choice of reference temperature given by Eq. (15), which leads to the simplified EOS of Eq. (16), the temperature of the CJ state is $T_{\text{cj}} = 2039$ K. The isotherm through the CJ state and the $T = 0$ isotherm are shown in figure 3. Several points are noteworthy:

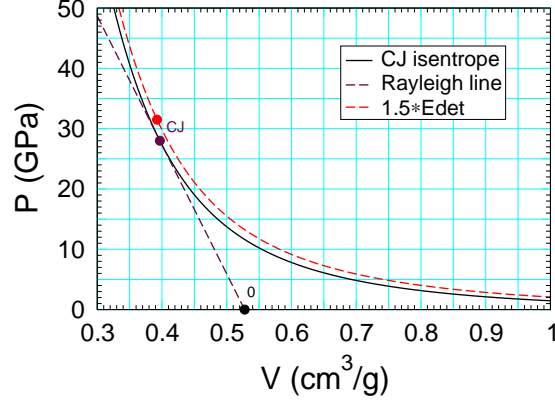


Figure 2: CJ isentrope and Rayleigh line. The initial state and CJ states are indicated by the circles.

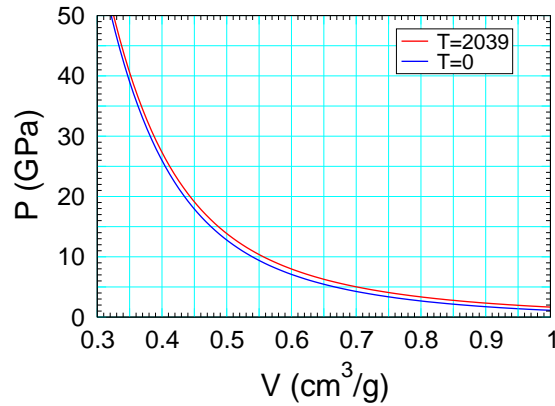


Figure 3: CJ isotherm and cold curve for products with simplified EOS, Eq. (16).

1. Explosive products are usually thought of as gaseous. However, the $T = 0$ isotherm is what one would expect for the cold curve of a solid. This is because the products are at high density and the EOS does not correspond to that of an ideal gas.
2. At the CJ state, the density is greater than the ambient solid density. One would expect the specific heat at such a high density to be close to the classical limit of a solid, which for TATB (the explosive component of PBX 9502) is $0.0023 \text{ MJ}/(\text{kg}\cdot\text{K})$. Despite C_v being much smaller, the CJ temperature is low; expect $T_{\text{cj}} = 3000$ to 4000 K . This is due to the high pressure of the “cold curve” at the initial density.
3. The pressure difference between the CJ isotherm and the cold curve is relatively small. This can cause problems with the P-T equilibrium mixture EOS of a partly burned explosive.

When the CJ temperature is chosen to be higher, Eqs. (13, 14) rather than Eq. (16), the low temperature isotherms are qualitatively different. Figure 4 shows selected isotherms for the EOS when T_{cj} is chosen to be 3500 K . There are two anomalies. First, the lowest isotherms ($T \lesssim 500 \text{ K}$) dip below zero pressure. Second, the isothermal compressibility goes negative, $K_T = -V(\partial_V P)_T < 0$, along portions of some isotherms. This occurs at $T = 500 \text{ K}$ even when the pressure is positive. Both anomalies limit the

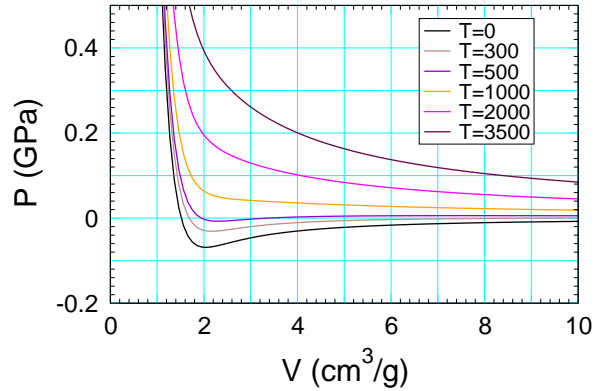


Figure 4: Low temperature isotherms in the expansion region ($V > V_0$) for products EOS with $T_{\text{cj}} = 3500 \text{ K}$.

domain of the EOS. In particular, the room temperature products isotherm ($T \approx 300$ K) is not entirely within the domain.

The anomalous behavior of the isotherms at low temperatures is not special to the JWL EOS. Rather it is typical of a Mie-Grüneisen form of EOS with a constant specific heat. Physically, the specific heat and the entropy should go to zero at $T = 0$. The Mie-Grüneisen EOS is compatible with a non-constant specific heat; see for example [Menikoff, 2009].

For the reactants, selected isotherms in the expansion region are shown in figure 5. Even at 700 K, when the pressure is positive, the expansion region is limited by the isothermal compressibility going negative. Qualitatively, the isotherm displays a van der Waal loop. Most EOS models for solids have similar issues in the expansion region. Physically, the difficulty is that the tacit assumption of a single phase EOS model breaks down; *i.e.*, sublimation leads to a mixed solid-vapor phase.

For an explosive, P - T equilibrium is frequently used for partly burned HE. Since P - T equilibrium requires the component EOS are thermodynamically stable, these examples show domain issues with the JWL EOS that can cause a P - T equilibrium solution to fail to exist; typically, for moderate temperature in expansion.

For a constant volume burn, the thermodynamic state corresponds to that of the products at (V_0, e_0) . The energy on the CJ isentrope at V_0 is less than e_0 by an amount equal to the area of the region in the (V, P) -

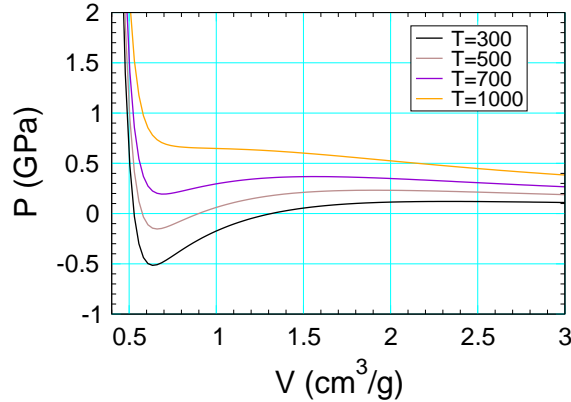


Figure 5: Selected isotherms in the expansion region ($V > V_0$) for reactant EOS.

plane between the CJ isentrope and the Rayleigh line over the interval $V_{\text{cj}} \leq V \leq V_0$. Consequently, the constant volume burn temperature and pressure are greater than the values on the CJ isentrope at V_0 , which we denote by T_{cvb} and $T_{\text{cj}}(V_0)$, respectively, and similarly for the pressure. For the example, $T_{\text{cvb}} = 2828$ K and $P_{\text{cvb}} = 12.2$ GPa compared to $T_{\text{cj}}(V_0) = 1768$ K and $P_{\text{cj}}(V_0) = 11.6$ GPa. It is anomalous for T_{cvb} to be so much greater than the CJ temperature of 2039 K. This indicates that T_{cj} is too low. However, raising T_{cj} would lead to the low temperature anomaly shown in figure 4. The trade-off in anomalies point to an inherent weakness in the thermal component of a Mie-Grüneisen EOS with a constant specific heat.

Typically, JWL parameters for explosive products are calibrated to data for the CJ release isentrope, and for explosive reactants to shock Hugoniot data. At pressures above the data, the JWL EOS represents an extrapolation and can loss accuracy. Figure 6 compares the shock locus and the overdriven detonation locus determined from the JWL EOS with experimental data. An anomalous feature of the plot is that the loci cross at a pressure just above the von Neumann spike state of a CJ detonation. Double shock experiments utilize an HE property, known as shock desensitization, to get higher pressure reactants data [Aslam, 2011]. These are compatible with a reactants EOS for which the reactants shock locus remains below the detonation locus.

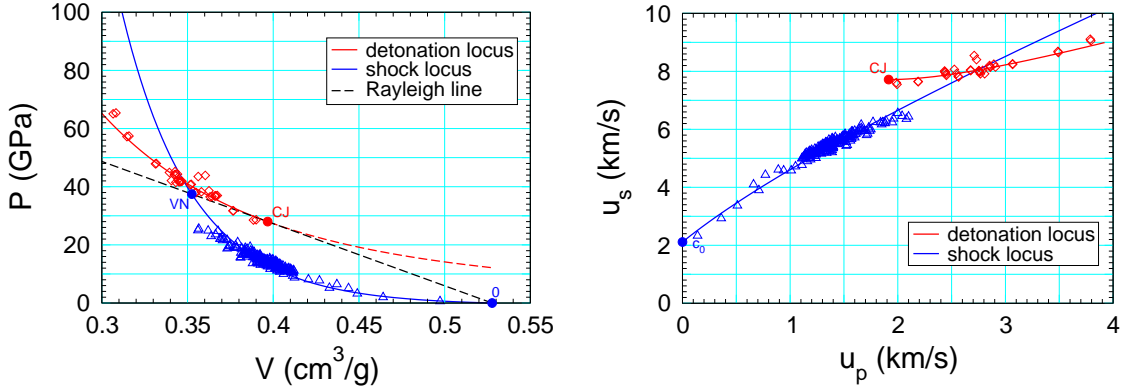


Figure 6: Comparison of shock locus and detonation locus from JWL EOS with data for PBX 9502. Shock data from [Dick, 1988; Gustavsen, 2006], and overdrive detonation data from [Tang, 1998; Green, 1985].

Exercise for the student

In the section on ‘heat of detonation,’ it was shown that the area between the CJ release isentrope and the Rayleigh line is the heat of detonation, which corresponds to the parameter Δe . With Δe set to 0 for the explosive products used in the previous section, figure 7 shows the CJ release isentrope and the Rayleigh line. Compared to figure 2 the detonation speed (slope of Rayleigh line) and the CJ pressure are lower. But the area does not appear to be zero. Explain the paradox.

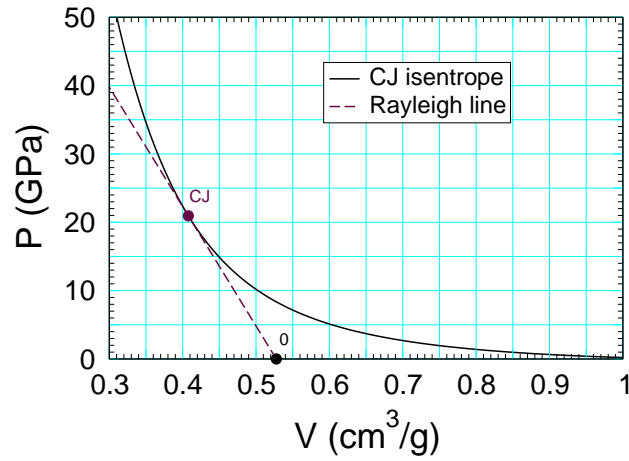


Figure 7: CJ isentrope and Rayleigh line for $\Delta e = 0$.

Resolution of paradox

For the CJ state, the isentrope parameter C is negative. Figure 8 shows the extension of the isentrope to the expansion region. For $V \gtrsim 1.1 \text{ cc/g}$, the pressure is negative. For the expansion portion of release isentrope with $P < 0$ the signed area between the isentrope and the P -axis is negative. Even though the negative pressure is small compared to the CJ pressure, the V interval with $P < 0$ is much larger than that with $P > 0$, and the positive and negative areas cancel.

If the domain of the EOS is limited to be the region of the (V, e) -plane with $P(V, e) > 0$, then the effective value of the heat release, $-\Delta H_{det}$ from Eq. (24) with $P_{final} = 0$, is greater than 0, and is consistent with figure 7.

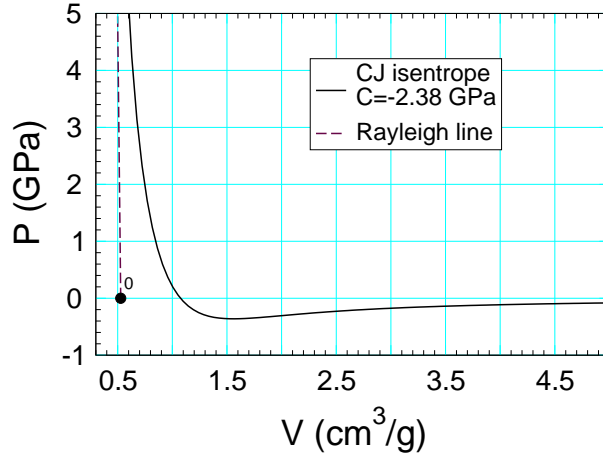


Figure 8: CJ isentrope for $\Delta e = 0$, expansion region.

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References

- T. D. Aslam, “*Double shock experiments and modeling of PBX 9502 reactants*,” presentation at conference Shock Compression of Condensed Matter (2011). <http://www.osti.gov/scitech/servlets/purl/1078411>
- J. J. Dick, C. A. Forest, J. B. Ramsay, and W. L. Seitz, “*The Hugoniot and shock sensitivity of a plastic-bonded TATB explosive PBX 9502*,” J. Appl. Phys., 63 (1988) pp. 4881–4888.
- 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 equation of state of the detonation products*,” in Eighth Symposium on Detonation (1985), pp. 587–595.
- R. L. Gustavsen, S. A. Sheffield, and R. R. Alcon, “*Measurements of shock initiation in the tri-amino-tri-nitro-benzene based explosive PBX 9502: Wave forms from embedded gauges and comparison of four different material lots*,” J. Appl. Phys., 99 (2006) 114907/17.
- J. W. Kury, E. L. Lee, H. C. Hornig, J. L. McDonnel, D. L. Ornellas, M. Finger, F. M. Strange and M. L. Wilkins, “*Metal Acceleration by Chemical Explosives*,” in Fourth Detonation Symposium (1965), pp. 3–13.
- E. L. Lee, H. C. Hornig and J. W. Kury, “*Adiabatic Expansion of High Explosive Detonation Products*,” Technical Report LLNL, UCRL-50422 (1968).
- R. Menikoff, “*Complete EOS for PBX 9502*,” technical report, LA-UR-09-06529, LANL, 2009. <http://www.osti.gov/bridge/servlets/purl/1043481/>
- R. Menikoff, “*Complete Mie-Grüneisen Equation of State*,” technical report, LA-UR-12-22592, LANL, 2012. <http://www.osti.gov/bridge/servlets/purl/1045381/>

- P. K. Tang, W. W. Anderson, J. N. Fritz, R. S. Hixson, and J. E. Vorthman, “*A study of the overdriven behaviors of PBX 9501 and PBX 9502,*” in Eleventh Symposium on Detonation (1998), pp. 1058–1064.
- C. M. Tarver and E. M. McGuire, “*Reactive Flow Modeling of the Interaction of TATB Detonation Waves with Inert Materials,*” in Twelve Detonation Symposium (2002), pp. 641–649.