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Explosive Products EOS: Adjustment for detonation speed and energy release

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Abstract

Propagating detonation waves exhibit a curvature effect in which the detonation speed decreases with increasing front curvature. The curvature effect is due to the width of the wave profile. Numerically, the wave profile depends on resolution. With coarse resolution, the wave width is too large and results in a curvature effect that is too large. Consequently, the detonation speed decreases as the cell size is increased. We propose a modification to the products equation of state (EOS) to compensate for the effect of numerical resolution; *i.e.*, to increase the CJ pressure in order that a simulation propagates a detonation wave with a speed that is on average correct. The EOS modification also adjusts the release isentrope to correct the energy release.

1 Introduction

An underdriven detonation wave is self-sustaining. For a planar detonation, the detonation speed and the state behind the detonation front are determined by the Hugoniot jump conditions and the sonic (CJ) condition. Consequently, the detonation state is determined by the ambient (reactant) state and the equation of state (EOS) of the explosive products. A key point is that an underdriven planar detonation wave is independent of the burn rate.

For a curved detonation wave, the Hugoniot jump conditions have a correction term due to the reaction-zone width. Moreover, the sonic point lies within rather than at the end of the reaction zone. A consequence of these two properties is that the detonation speed and the release isentrope behind the detonation front depend on the front curvature and on the burn rate. This dependency is known as the curvature effect, though it is typically associated with the $D_n(\kappa)$ relation for the dependence of the detonation speed on front curvature.

The reaction-zone width depends on the burn rate for the explosive. For simulations, the reaction-zone width also depends on resolution. In particular, the numerical reaction-zone width increases as the resolution is coarsened. Since the leading order correction to the jump conditions is proportional to the (wave width)×(front curvature), the numerical resolution affects the curvature effect. Typically, the detonation speed decreases with coarser resolution.

A conventional high explosive (HE), such as PBX 9501, has a small reaction-zone width (less than 0.1 mm) and hence a small curvature effect. Resolving the reaction zone would require a cell size of 0.010 mm or less. Simulations typically use much coarser resolution. A recent resolution study [Menikoff, 2014] found for cylinder test simulations of PBX 9501 with the SURF burn model that the detonation speed and release isentrope varied by only 1 % over a wide range of cell sizes; from fine resolution (15 cells in reaction zone) to very coarse resolution (1 or 2 cells). The coarse resolution corresponds to using a burn rate to capture the detonation front (abrupt transition of reactants to products) in the same sense that numerical dissipation is used to capture a shock front (abrupt rise in pressure); *i.e.*, the wave profile in both cases is artificial with a larger width than physical.

The small change in the detonation speed and the release isentrope is likely related to the extremum properties of the planar CJ state; namely, on the detonation locus the CJ state corresponds to a local minimum in both the detonation speed and the entropy (hence release isentrope). The insensitivity to even coarse resolution implies an insensitivity to burn rate. This is what enables the programmed burn model and detonation shock dynamics model to work; *i.e.*, to have a small error in the release isentrope with coarse resolution and an artificial pseudo-rate.

When the errors in propagating a detonation wave from numerical resolution are small and within the calibration uncertainty of the HE model, it is natural to try and tweak the explosive EOS to compensate for systematic effects of resolution; *i.e.*, reaction-zone cell size. In the following sections we present a procedure for modifying the products EOS in a thermodynamically consistent manner in order to adjust the detonation speed and the energy release. While this can improve the accuracy of a simulation in some respects, such a methodology has inherent limitations. Adjusting the EOS can not compensate for the full curvature effect; *i.e.*, the $D_n(\kappa)$ relation. It can be used to get the average front speed for a particular application. Similarly, adjusting the energy release of the detonation isentrope can get the average push on a confining material, but not the full time history.

2 EOS

A complete thermodynamically consistent EOS can be defined by a Helmoltz free energy, F;

$$F(V,T) = e - T\,S \ , \tag{1a}$$

$$P(V,T) = -\partial_V F(V,T) \ , \tag{1b}$$

$$S(V,T) = -\partial_T F(V,T) \ , \tag{1c}$$

where V, T, e, P and S are the specific volume, temperature, specific energy, pressure and entropy, respectively.

To adjust the detonation state we will modify the products EOS by shifting the cold curve. This can be expressed as a temperature independent shift in the free energy;

$$\widetilde{F}(V,T) = F(V,T) + \Delta e_c(V) \ . \tag{2}$$

It follows from the thermodynamic relations that

$$\widetilde{P}(V,T) = P(V,T) + \Delta P_c(V)\ , \tag{3a}$$
$$\widetilde{S}(V,T) = S(V,T)\ , \tag{3b}$$

where $\Delta P_c(V) = -(\mathsf{d}/\mathsf{d}V)\Delta e_c(V)$. Moreover, the specific heat and the Grüneisen coefficient as a function of (V,T),

$$C_V(V,T) = T(\partial_T S)_V\ , \tag{4}$$
$$\Gamma(V,T) = -(V/T)\,(\partial_V T)_S = \frac{V\,(\partial_V S)_T}{T(\partial_T S)_V}\ , \tag{5}$$

are unchanged. The isentropes for the modified EOS are simply related to the original EOS;

$$\widetilde{T}_S(V) = T_S(V)\ , \tag{6a}$$
$$\widetilde{P}_S(V) = P_S(V) + \Delta P_c(V)\ , \tag{6b}$$
$$\widetilde{e}_S(V) = e_S(V) + \Delta e_c(V)\ . \tag{6c}$$

We will use the subscript 'CJ' to denote a quantity at the CJ state; *e.g.*, $P_{\rm CJ} = P(V_{\rm CJ}, e_{\rm CJ})$. On a function of V, the subscript 'CJ' will denote the quantity on the isentrope through the CJ state; *e.g.*, $P_{\rm CJ}(V) = P_{S_{\rm CJ}}(V)$ and $P_{\rm CJ} = P_{\rm CJ}(V_{\rm CJ})$.

The detonation speed $D_{\rm CJ}$ and CJ state ($V_{\rm CJ}$, $e_{\rm CJ}$, $P_{\rm CJ}$) of the original EOS are determined by the Hugoniot equation and the sonic condition:

$$e_{\rm CJ} = e_0 + \tfrac{1}{2}\,(P_{\rm CJ} + P_0)\cdot(V_0 - V_{\rm CJ})\ , \tag{7}$$
$$\frac{P_{\rm CJ} - P_0}{V_0 - V_{\rm CJ}} = -\Big(\frac{\partial P}{\partial V}\Big)_S\Big(V_{\rm CJ}, e_{\rm CJ}\Big) \equiv (D_{\rm CJ}/V_0)^2\ . \tag{8}$$

where (V_0, e_0, P_0) is the ambient reactants state.[1] Then the isentrope through the CJ state is determined by integrating the ODE

$$\mathsf{d}e/\mathsf{d}V = -P(V,e)\ , \tag{9}$$

[1] If the HE model has an explicit energy release Q in addition to an offset in the energy origins of the reactants and products, then e_0 in the Hugoniot equation (7) should be replaced by $e_0 + Q$.

with the initial condition $e(V_{\rm CJ}) = e_{\rm CJ}$. We note, the sonic condition has the geometric interpretation that the CJ isentrope is tangent to the Rayleigh line; $P = P_0 - P'_{\rm CJ}(V_{\rm CJ})(V_0 - V)$.

The problem is to determine $e_c(V)$ such that the modified EOS has a small shift in the detonation speed and in the energy release;

$$\widetilde{D}_{\rm CJ} = D_{\rm CJ} + \Delta D \ , \tag{10}$$

$$\tilde{e}_{\rm CJ} - \tilde{e}_{\rm CJ}(V_*) = [e_{\rm CJ} - e_{\rm CJ}(V_*)] + \Delta e \ , \tag{11}$$

where V_* is some suitable value of the specific volume in expansion that is relevant to an application, such as the rule of thumb $V_* = 7\,V_0$.

We choose the new CJ state to be $(V_{\rm CJ}, P_{\rm CJ} + \Delta P_{\rm CJ})$. We note that it has the same specific volume as the original EOS, and that the change in the detonation speed is

$$\begin{aligned} \frac{\Delta D}{V_0} &= \left[\frac{P_{\rm CJ} + \Delta P_{\rm CJ} - P_0}{V_0 - V_{\rm CJ}}\right]^{1/2} - \left[\frac{P_{\rm CJ} - P_0}{V_0 - V_{\rm CJ}}\right]^{1/2} \\ \frac{\Delta D}{D_{\rm CJ}} &\approx \tfrac{1}{2}\,\frac{\Delta P_{\rm CJ}}{P_{\rm CJ} - P_0} \ . \end{aligned} \tag{12}$$

Moreover, the CJ isentrope determines the shift in the cold curve; *i.e.*, $\Delta P_c(V) = \Delta P_{\rm CJ}(V)$.

The energy shift can then be expressed in terms of the pressure shift on the CJ isentrope:

$$\Delta e_c(V) = \Delta e_{\rm CJ} - \int_{V_{\rm CJ}}^{V} \mathsf{d}V' \Delta P_{\rm CJ}(V') \ , \tag{13a}$$

$$\Delta e_{\rm CJ} = \tfrac{1}{2}\,\Delta P_{\rm CJ} \cdot (V_0 - V_{\rm CJ}) \ . \tag{13b}$$

The choice of $\Delta e_{\rm CJ}$ guarantees that the new CJ state lies on the detonation locus of the modified EOS.

We construct $\Delta P_c(V)$ separately in two regions: $0 \le V \le V_0$ and $V_0 < V$. Continuity of ΔP_c and its first and second derivatives are required in order that the release wave does not have kinks or a split wave structure; *i.e.*, the characteristic velocity varies smoothly with pressure.

Region 1: $0 < V \le V_0$

In this region we take $\Delta P_{\rm CJ}(V)$ to be linear;

$$\Delta P_{\rm CJ}(V) = \Delta P_{\rm CJ} \cdot (V_0 - V)/(V_0 - V_{\rm CJ}) \ . \tag{14}$$

This satisfies the sonic condition for the new CJ state;

$$\begin{aligned}
-\Big(\frac{\partial \widetilde{P}_{\rm CJ}}{\partial V}\Big)\big(V_{\rm CJ}\big) &= -\Big(\frac{\partial P_{\rm CJ}}{\partial V}\Big)\big(V_{\rm CJ}\big) - \Big(\frac{\partial \Delta P_{\rm CJ}}{\partial V}\Big)\big(V_{\rm CJ}\big) \\
&= \frac{P_{\rm CJ} - P_0}{V_0 - V_{\rm CJ}} + \frac{\Delta P_{\rm CJ}}{V_0 - V_{\rm CJ}} \\
&= \frac{\widetilde{P}_{\rm CJ} - P_0}{V_0 - V_{\rm CJ}} \ .
\end{aligned}$$

We also note that $\Delta P_{\rm CJ}(V_0) = 0$ and $\Delta P_{\rm CJ}(V) \ge 0$. Hence, it gives a positive contribution to the shift in the energy release. Asymptotically $\Delta P_{\rm CJ}(0) = \Delta P_{\rm CJ} \cdot V_0/(V_0 - V_{\rm CJ})$ is negligible since $P_{\rm CJ}(V) \to \infty$ as $V \to 0$.

Region 2: $V_0 < V$

In this region we take $\Delta P_{\rm CJ}(V)$ to be proportional to $P_{\rm CJ}(V)$;

$$\Delta P_{\rm CJ}(V) = -f(V)[1 + a\, f(V)]\, \frac{V_0}{V_0 - V_{\rm CJ}} \cdot \frac{\Delta P_{\rm CJ}}{P_{\rm CJ}(V_0)}\, P_{\rm CJ}(V) \ , \tag{15a}$$

$$f(V) = \frac{1 - V_0/V}{1 + [(V/V_0 - 1)/dv]^2} \ , \tag{15b}$$

where a and dv are dimensionless parameters. We note that $f(V) \ge 0$ for $V > V_0$, $f(V_0) = 0$ and $f(V) \to 0$ as $V \to \infty$. Independent of the parameters, $\Delta P_{\rm CJ}(V)$ and its first derivative at V_0 match the values in region 1 at V_0. The parameter a is chosen such that the second derivative is 0 at V_0; *i.e.*, matches second derivative in region 1. Straight forward algebra yields

$$a = 1 - V_0\, P'_{\rm CJ}(V_0)/P_{\rm CJ}(V_0) \ . \tag{16}$$

Since the slope of an isentrope is negative, $P'_{\rm CJ} = (\mathsf{d}/\mathsf{d}V)P_{\rm CJ}(V) < 0$ and the parameter a is positive. Hence, $\Delta P_{\rm CJ}(V) \le 0$. The parameter dv controls how fast $f(V)$ goes to 0. Since $f(V)$ is monotonically decreasing with decreasing dv, it can be used to adjust the energy release.

3 Illustrative example

As an example of the modified EOS construction, we take the original CJ isentrope to be $P_{\text{CJ}}(v) = 30\, v^{-\gamma}\,\text{GPa}$, where $\gamma = 3$ where $v = V/V_{\text{CJ}}$. Furthermore, we take $v_0 = V_0/V_{\text{CJ}} = 1.3$. This roughly corresponds to a solid HE, such as PBX 9501 or PBX 9502. Typically, P_{CJ} has an uncertainty of few tenths of GPa.

For the adjusted CJ pressure we take $\Delta P_{\text{CJ}} = 0.5\,\text{GPa}$. This corresponds to $\Delta D/D_{\text{CJ}} = 0.8\,\%$. For the modified products EOS, $\Delta P_{\text{CJ}}(V)$ is shown in figure 1 for several choices of the parameter dv. We note that the shift in the energy release,

$$\Delta e = \int_{V_{\text{CJ}}}^{V_*} \mathsf{d}V'\, \Delta P_{\text{CJ}}(V')\ , \tag{17}$$

decreases with increasing dv. It may be either positive or negative. For the example, $\Delta e = 0$ corresponds to $dv = 0.26$.

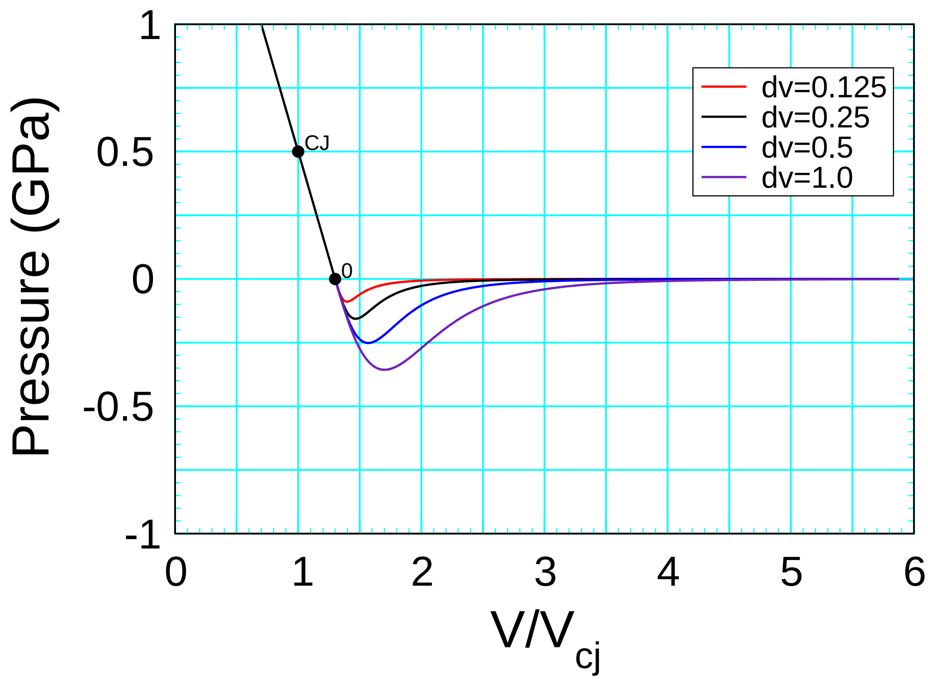

Figure 1: Shift in cold curve pressure, ΔP_c, as parameter dv is varied.

4 Final remarks

Modification of the products EOS to adjust the detonation speed and energy release is not unique. The construction here is general in that it makes no special assumptions on the EOS. Furthermore, it maintains the asymptotic behavior of the original EOS as $V \to 0$ and $V \to \infty$.

The last requirement, $\Delta P_{\text{CJ}}(V) \to 0$ as $V \to \infty$, forces $\Delta P_{\text{CJ}}(V)$ to be non-convex, as seen in figure 1. For the release wave behind a detonation to be a rarefaction wave, the modified CJ isentrope, $\widetilde{P}_{\text{CJ}}(V) = P_{\text{CJ}}(V) + \Delta P_{\text{CJ}}(V)$, needs to be convex. This limits ΔP_{CJ} and hence the detonation speed and energy release adjustments to be small.

In addition, there maybe restrictions on the domain. Typically, products EOS are of the Mie-Grüneisen form with a constant specific heat. Since $C_V \not\to 0$ as $T \to 0$, isotherms at low temperatures have van der Waal loops. Detonation waves are at high pressure and high temperature ($T > 1000\,\text{K}$). The flow for detonation simulations typically does not get into the anomalous region. But such an EOS model would not be appropriate for deflagration waves with initial state around room temperature.

References

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