



Scaling of the detonation product state with reactant kinetic energy

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ABSTRACT

Chemical explosives provide one of the most high-power and energy-dense storage materials available. During detonation, transfer of this energy to adjacent materials is governed by the detonation product equation of state. No accurate methodology exists for prediction of this thermodynamic relationship and equation-of-state data continues to be experimentally characterized for each new formulation or charge density. Here we present a universal detonation product equation of state derived from several newly discovered empirical correlations in prior condensed-phase detonation product measurements. This model depends only on initial charge density and detonation velocity as inputs, dramatically simplifying the calibration process relative to existing models, which require measurement of up to seven formulation-specific parameters. This new result implies the product energy density scales with reactant kinetic energy density, which is the product of the explosive initial density and detonation velocity squared, for all condensed-phase energetic materials and that explosive microstructural or chemical details only influence the product energy density through these two parameters.

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1. Introduction

Detonating condensed-phase explosives produce product energy densities approaching 14 MJ/L and energy release rates exceeding 1 TW/m², which is higher than the radiative flux at the solar surface. Despite extensive use in the mining and defense industries for several centuries, no accurate methodology exists for prediction of the detonation product equation of state (EOS), which governs the transfer of energy from the products to adjacent materials. This work is typically achieved through pressure–volume expansion of the detonation products, as their high pressure exceeds the yield strength of all known materials. The product EOS and detonation velocity D_0 , constitute the two most important parameters to designers of explosive systems. Efforts to theoretically or empirically unify all explosive product measurements have had only limited success [1–6].

Models have also been developed to estimate D_0 and product EOS parameters from thermochemical equilibrium assumptions [7,8]. While these models are continually being improved, they rely heavily on assumed reaction zone kinetics and detonation product species that are not directly measured or known for most high explosive detonation flows. Instead, they are empirically calibrated to existing D_0 , EOS data, and assumed final product states, which can be insufficient to fully constrain their predictions. Thus, equation-of-state data continues to be experimentally characterized for each

new formulation, charge density and scale, which requires an expensive and specialized series of tests and analysis [9].

Measurement of the product EOS and D_0 can prove challenging as they vary locally in a charge depending on formulation, density, scale, and shape variation. Additionally, the product states behind the detonation wave are extreme, approaching 40 GPa and 4000 K with significant optical opacity. These conditions render conventional thermodynamic-sensing flow diagnostics useless and advanced light source test facilities cannot yet accommodate large enough charges to recreate the detonation reaction zone conditions present in engineering-scale explosive systems. Thus, traditional explosive product EOS measurement techniques continue to involve detonation of large metal-confined charges and infer the product EOS from the resulting high-rate metal deformation. Prior to this work, each explosive EOS measurement has been considered distinct with no capability to relate EOS's from different explosive formulations or densities to one another.

Here, the discovery of a universal EOS for detonation products is reported that is based on the identification of multiple empirical correlations in product EOS data that have not been previously observed. This common product model utilizes only two material-specific measurable parameters, the explosive initial density ρ_0 and D_0 , to predict the detonation product isentrope. This approach is a dramatic simplification of current EOS models that rely on seven or more parameters, many of which cannot be directly measured. The existence of this common product model, which approximates the product state of all known condensed-phase explo-

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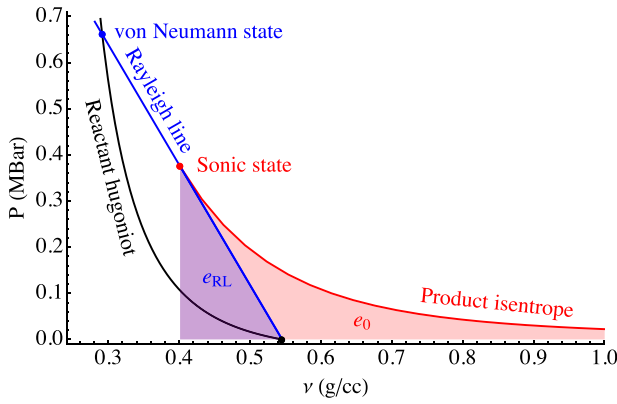


Fig. 1. Thermodynamic paths relevant to detonation in P - v space for PBX 9501 explosive. Reactant Hugoniot, Rayleigh line, and product isentrope are black, blue, and red curves, respectively. The initial, von Neumann, and sonic states are represented by the black, blue, and red points, respectively. The red shading represents e_0 , overlapping blue shading representing e_{RL} , and $\Delta h_d = e_0 - e_{RL}$. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

sives, implies that, to leading order, the explosive product EOS is independent of microstructure and chemical details.

2. Background

In a steady detonation, shock passage through an explosive adiabatically compresses the metastable reactants and induces onset of exothermic chemical reaction. The energy release then is thought to drive the reacting flow to a locally sonic state, which isolates the reaction zone from downstream perturbations. Of the total chemical energy released e_0 , a portion referred to here as the Rayleigh energy e_{RL} is used to support the shock wave's mechanical compression of the reactants and the remainder is the heat of detonation Δh_d , which is stored in the products as internal or kinetic energy. For one-dimensional flow, the thermodynamic path of the detonation is shown in Fig. 1. Shock compression drives the explosive to the von Neumann state defined by the intersection of the Rayleigh line and the reactant Hugoniot. Chemical reaction then expands the flow down the Rayleigh line to the sonic state, where the product Hugoniot is tangent to the Rayleigh line. (The Chapman–Jouguet and sonic states are identical for one-dimensional flow.) The flow subsequently expands down the product isentrope in the absence of any additional shocks. Material is defined as reactant when it is upstream of the shock, reaction zone flow when it is between the shock and sonic surface, and products when it is downstream of the sonic surface. Additional flow dimensionality does not alter these physics qualitatively, but does allow for a flow component normal to the shock, which can result in transversely varying thermodynamic properties.

In practice, the product parameters are inferred from an experimental cylinder expansion test that consists of a ductile metal tube filled with explosive [10]. After explosive detonation, the tube wall is accelerated by the products. Knowledge of the explosive initial density ρ_0 and measurement of the detonation velocity D_0 yield the Rayleigh line, while analysis of the tube motion with a computational or analytical hydrodynamic model is used to infer the product isentrope along with the thermodynamic state of the sonic point [9,11,12]. (During this analysis, the detonation is generally approximated as one-dimensional, thus yielding a single sonic state.) Isentropes are then fit to an analytic EOS form, typically the JWL (Jones–Wilkins–Lee) EOS, for concise presentation [11].

The JWL is an incomplete EOS developed for use with condensed-phase explosive products [11]. Consisting of the sum of three functions that are dominant at different product volumes and yielding perfect gas behavior ($Pv^{1+\omega} = \text{constant}$) at lower pressures, the JWL pressure equation on the principle isentrope is

$$P(\Lambda) = Ae^{-R_1\Lambda\Delta_s} + Be^{-R_2\Lambda\Delta_s} + C(\Lambda\Delta_s)^{-(1+\omega)}$$

where $\Delta_s = v_s/v_0$ and $\Lambda = v/v_s$ with v as the specific volume, v_s denoting the sonic state condition, and $v_0 = 1/\rho_0$. We have introduced Λ via the algebraic expansion $\Delta = \Lambda\Delta_s$ where $\Delta = v/v_0$ to later plot JWL data at volumes relative to those of the sonic state.

Pressure is related to the energy on the isentrope I by

$$\left(\frac{\partial e}{\partial \Lambda}\right)_I = \Delta_s \left(\frac{\partial e}{\partial \Delta}\right)_I = -\Delta_s P \quad (1)$$

with e as the energy density or energy per unit volume, which is dimensionally equivalent to pressure. The product energy along the principle isentrope is thus

$$e(\Lambda) = \frac{A}{R_1}e^{-R_1\Lambda\Delta_s} + \frac{B}{R_2}e^{-R_2\Lambda\Delta_s} + \frac{C}{\omega}(\Lambda\Delta_s)^{-\omega}.$$

These equations can also be utilized with the Grüneisen parameter to generate thermodynamic conditions away from the principle isentrope [11,13].

The JWL equations have eight calibration parameters, five of which are dimensional (A , B , C , v_s , and v_0) and three of which are nondimensional (R_1 , R_2 , and ω). Cylinder expansion data is usually valid to $\Delta < 10$ and $P \approx 0.001$ MBar, which is sufficient to constrain the A , B , R_1 , R_2 , and v_s terms. Parameter v_0 is measured before testing. Thermochemical equilibrium calculations or detonation calorimetry measurements are generally used to constrain the C and ω terms [11,14]. Calibration parameters of the JWL for many different explosives, as derived primarily from cylinder expansion tests, are available in published literature with many reproduced in Table A.3. In general, they are able to predict cylinder wall expansion velocities to within $\pm 0.5\%$ [11]. The Davis EOS is also less commonly used to fit detonation product EOS data and involves a similar number of calibration parameters [15].

3. Product parameter scaling

Figure 2 plots Δh_d and e_{RL} as determined in previous work for many explosive formulations versus $S = \rho_0 D_0^2$, the kinetic energy of the reactants in the shock frame. The filled circles represent Δh_d measured by detonation calorimetry in 12.7-mm-diameter charges [14,16]. Ornellas [16] only measured Δh_d and we have paired this data with D_0 values corrected for charge size, density, and confinement as determined from separate sources using similar scale tests. The calorimetry data and sources are listed in Table A.2. The crosses denote Δh_d values and the triangles are their corresponding e_{RL} values, as derived from JWLs primarily calibrated to cylinder tests, including those listed in Table A.3. The e_{RL} data is seen to follow a strong linear trend in S . The Δh_d trend is approximately \sqrt{S} at low values and S^1 at the largest measured values. The experimental calorimetry data exhibits relatively little scatter in comparison to the Δh_d JWL data, whose Δh_d value is highly dependent on thermochemical equilibrium assumptions for the product species. In this sense, calorimetry measurements provide a more direct estimate of Δh_d .

Such relationships have not been previously recognized and imply that both Δh_d and e_{RL} scale with S across all explosive formulations, to leading order. Secondary effects are also apparent with two explosives classes deviating from the trend. Insensitive explosives, composed of TATB and LLM-105 base molecules, are low relative to the global data trend for both Δh_d and e_{RL} . Aluminized explosives exhibit substantial scatter, but trend to higher Δh_d .

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