Validation of a High Explosive Detonation Product Equation of State via a Slab Geometry Test

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1 Introduction

A detonation in a high explosive (HE) generates large pressures (up to a few 10s of GPa) due to a rapid energetic shock-driven combustion process [1–3] in the condensed phase HE. The energy accumulated by the products of detonation is then available to provide push on the surrounding HE confinement as the products expand volumetrically. Thus, accurately calibrated models of the detonation products equation of state (EOS) are essential for typical HE applications. Such EOSs are normally calibrated from data obtained in a cylinder expansion (CYLEX) test [4, 5]. In the CYLEX experiment, a cylinder of HE with a large aspect ratio is encased in a thin-walled, annealed, copper (Cu) tube. The velocity component of the outer wall of the expanding Cu tube is measured as the HE is detonating in a steady-state motion. This expansion data is then used to calibrate the parameters of a given form of detonation product EOS. By far the most commonly calibrated detonation product EOS model is the Jones-Wilkins-Lee (JWL) form. Calibrations of the product JWL EOS have been obtained for a large number of HEs, including cyclotrimethylenetrinitramine (RDX), cyclotetramethylene-tetranitramine (HMX), triamino-2,4,6-trinitrobenzene (TATB) and ammonium nitrate based materials [4, 6–9].

A variety of JWL EOS calibration methods have been developed based on data obtained in the CYLEX test configuration, with the majority involving hydrodynamic simulations based on programmed burn (PB) calculations [4, 6, 10]. In recent work [9, 11, 12], the present authors have developed a sophisticated methodology for calibrating the JWL EOS of detonation products via CYLEX tests. It involves the use of a PB approach employing accurate detonation timing calculations via velocity-curvature detonation shock dynamics (DSD) modeling, combined with velocity-adjusted JWL EOS hydrodynamic simulations of the Cu CYLEX wall motion driven by the expanding HE detonation products. The EOS parameters are iterated on over the course of several hundreds of hydrodynamic simulations, until the complete experimental Cu wall expansion trajectory is reproduced to within some predefined metric [9]. However, to date, there has been little attention paid to the validation of the JWL product EOSs derived from CYLEX geometry tests. In particular, the ability to demonstrate the predictive capability of HE models calibrated in one geometry and then applied to other geometries is an essential component of HE detonation modeling [13].

In the following, we describe a slab expansion (SLABEX) test [14, 15] to provide such a validation of the CYLEX test-based calibration process for the JWL detonation products EOS developed in [9, 11,

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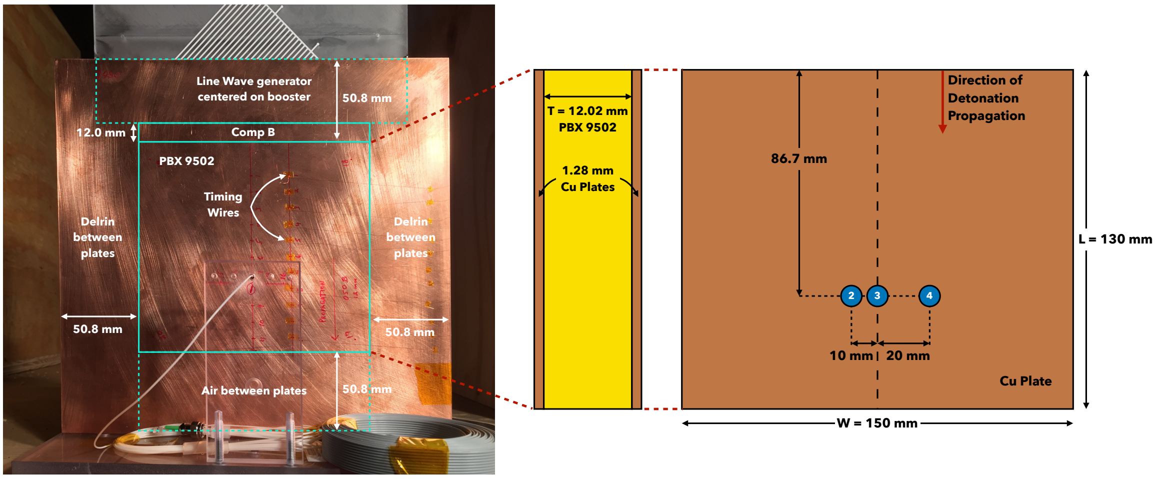

Figure 1: (a) Image of the top view of the T = 12.02 mm SLABEX test, with annotations showing the positions of the various inner materials between the Cu plates. (b) Side view of the PBX 9502 slab confined by the Cu plates. (c) Position of PDV probes 2-4 relative to the surface of one of the Cu plates covering the PBX 9502 slab. PDV probe 1 is situated at the same position as probe 3 on the other plate.

Table 1: Geometry data for the SLABEX test (see Fig. 1). T is the thickness of the PBX 9502 slab, Cu IT represents the distance between the inner surfaces of the Cu plates, while Cu OT is the corresponding distance between the outer surfaces of the Cu plates. The density of the PBX 9502 slab is given by ρ_0, while D_0 is the measured steady detonation speed.

T (mm)	Cu IT (mm)	Cu OT (mm)	ρ_0 (g/cm^3)	D_0 (mm/μs)	Std. Error D_0 (m/s)
12.02	12.06	14.62	1.888	7.562	1.33

12]. The SLABEX test consists of a rectangular slab of PBX 9502, a polymer-bonded HE formulation consisting of 95 wt.% 1,3,5-triamino-2,4,6-trinitrobenzene (TATB) bound with Kel F-800, a co-polymer of chlorotrifluoroethylene and vinylidene-fluoride. Hydrodynamic simulations of the Cu plate expansion in the SLABEX geometry are then conducted using the JWL product EOS for PBX 9502 recently calibrated in the CYLEX test geometry [9], and compared to the measured lateral component of the velocity of the expanding Cu plates in the SLABEX experiment.

2 Experimental SLABEX test

The SLABEX test geometry is described in Fig. 1. The test consists of a rectangular slab of PBX 9502, specifically virgin lot HOL88H891–008 (lot 008), with thickness T=12.02 mm, length L=130 mm, and width W=150 mm, giving L/T $\approx$ 11. The slab is confined by annealed Cu plates of thicknesses 1.28 mm. The silcone elastomer Sylgard is used to bond the Cu plates to the PBX 9502 slab assembly. A line wave generator is used to uniformly initiate a detonation in a booster, which subsequently initiates a detonation in the PBX 9502 slab.

On one of the Cu plates, three PDV probes were placed at a distance of 2/3L (86.7 mm) from the leading, booster-attached edge of the PBX 9502 slab (Fig. 1). One of the probes was offset from the central axis by 10 mm and the other by 20 mm, as shown, to ensure that the flow remains 2D near the central axis for the duration of the test. On the other Cu plate, a single probe was positioned at the equivalent location of the central axis probe in Fig. 1. Additionally, the measured steady detonation speed D_0 for the SLABEX test is given in table 1.

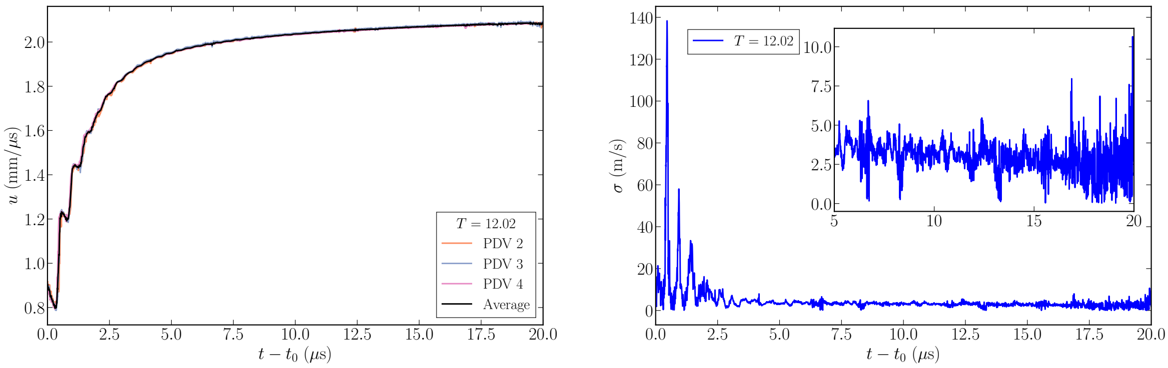

Figure 2: Measurement of the lateral components of velocity of the outer surfaces of the Cu plates (u) with time (t) relative to the time of wall motion start (t_0) for the various PDV probes shown (see Fig. 1). Also plotted is the velocity-time trace of the averaged PDV probe data. The figure on the right shows the standard deviation of the velocity traces from the average.

The time-varying lateral component of velocity of the outer surfaces of the Cu plates, plotted relative to the time of wall motion start, is shown in Fig. 2 for the SLABEX test, along with an average of the data obtained as in [9]. One probe (probe 1) did not return usable data. Figure 2 also shows the standard deviation of the velocity traces from the average, showing that the deviation is within 10 m/s after the early stages of ringing in the Cu plates. Moreover, the overlap of the off-center traces (from the PDV probes labeled 2 and 3 in Fig. 1) with the central axis trace shows that the flow evolution near the central axis of the slab remains 2D for the duration of the test.

3 Calibration of the detonation product JWL EOS from a CYLEX test geometry

For JWL EOSs, the Mie-Grüneisen form is given by

$$p = A\left(1 - \frac{\omega v_0}{R_1 v}\right)\exp\left[-R_1 v/v_0\right] + B\left(1 - \frac{\omega v_0}{R_2 v}\right)\exp\left[-R_2 v/v_0\right] + \frac{\omega e}{v}, \tag{1}$$

where p is the pressure, v is the specific volume and v_0 $(= 1/\rho_0)$ is the initial specific volume of the HE, and A, R_1, B, R_2 and ω are the JWL EOS parameters. In [9], we conducted a CYLEX geometry test on PBX 9502 lot 008 for the purposes of calibration of Eqn. (1). Specifically, a cylinder of PBX 9502 with diameter 25.43 mm was inserted into a Cu tube of inner diameter 25.44 mm and outer diameter 30.49 mm. The density of the PBX 9502 lot 008 was 1.891 g/cm^3, and the measured steady detonation speed was 7.582 mm/μs. The velocity of the outer surface of the expanding Cu tube was measured at various locations and tube orientations, and an average trajectory calculated (as plotted in Fig. 3a). In order to calibrate the JWL EOS for the PBX 9502 detonation products, the CYLEX experiment is simulated in a Lagrangrian hydrocode [16] using a programmed burn (PB) simulation method. The HE PB timing component for the CYLEX simulation uses the calibrated lot 008 detonation shock dynamics model (DSD) calculated in [9]. The corresponding HE PB energy release component is calculated through a velocity-adjusted JWL method. The Cu confiner in the CYLEX simulation is modeled with a tabular EOS [17], together with the plastic deformation model and its Cu parameterization defined in [18]. The starting mesh resolution was 62.5 μm based on a uniform grid, which we verified to be sufficient to ensure grid-converged solutions of the CYLEX test simulation with the PB model.

The JWL EOS model parameters A, B, R_1, R_2 and ω are then calibrated via the CYLEX experiment using a Nelder-Mead merit function minimization approach. Specifically, for a given set of EOS parameters, the simulated and experimentally measured Cu wall radial expansion profiles are compared, and

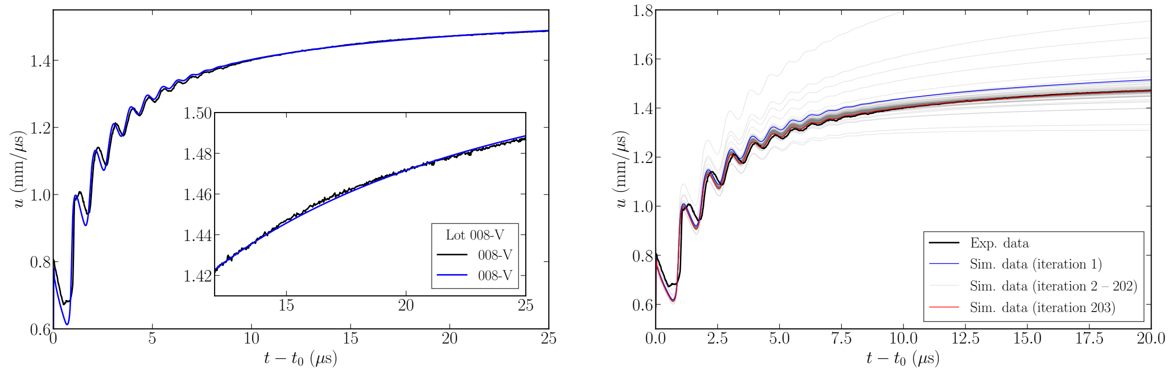

Figure 3: (a) Comparison of the averaged experimental and simulated motion of the outer surface of the Cu tube for the CYLEX test geometry, with the simulation based on the final PBX 9502 lot 008 JWL EOS model (Eqn. 1 and table 2). (b) Comparison of the experimental Cu wall motion with the CYLEX simulation at various stages in the EOS parameter iteration sequence. The black line represents the experimental measured motion, the blue line is from the CYLEX simulation for the starting EOS parameters, grey lines are simulation trajectories during the iteration sequence, and the red line is the final simulation for the fully calibrated parameters.

Table 2: JWL product EOS parameters for PBX 9502 lot 008 with the corresponding heat of detonation e_0 for $D_{CJ} = 7.8$ mm/μs [9].

A (GPa)	B (GPa)	R_1	R_2	ω	ρ_0 (g/cm^3)	e_0 (mm^2/μs^2)
698.7453	16.8548	4.5737	1.6576	0.3196	1.891	3.8515

A, B, R_1, R_2 and ω are then iterated on to provide the desired level of fit. Various stages in the iteration sequence are shown in Fig. 3b as A, B, R_1, R_2 and ω evolve. Table 2 shows the final JWL product EOS parameters A, B, R_1, R_2 and ω obtained from the minimization process over two hundred iterations (simulations), along with the corresponding heat of detonation e_0, which enforces a Chapman-Jouguet speed of $D_{CJ} = 7.8$ mm/μs for consistency with the DSD-based timing model.

4 Prediction of Cu plate expansion for the SLABEX geometry and comparison to experimental data

The SLABEX experiment described in §2 is simulated using the same methodology as for the CYLEX geometry simulations described above, but now using the parameterization for PBX 9502 lot 008 JWL EOS shown in table 2. The starting mesh resolution was 40 μm based on a uniform grid, which we have again verified is sufficient to ensure grid-converged solutions of the SLABEX test simulation.

Figure 4 shows a comparison of the averaged experimental and the simulated motion of the outer surface of the Cu plates for the SLABEX test geometry (T $= 8.04$ mm). Also shown are the relative velocity differences between the experiment and simulation with time. The simulation captures the experimental data well, with maximum velocity differences of $O(10-20)$ m/s after the early ringing stages in the Cu plate motion. Of note is that the initial ringing behavior in the motion of the Cu plates in the SLABEX test (as observed in Fig. 4), resulting from detonation-induced compressible wave reflections between the inner and outer surfaces of the Cu plates, is moderately well captured by the SLABEX geometry simulation. This could possibility indicate that Cu spall plays a lesser role in the SLABEX geometry than the CYLEX geometry. Overall, the results shown in Fig. 4 offer more than satisfactory validation of our advanced calibration process for the detonation products equation of state (EOS).

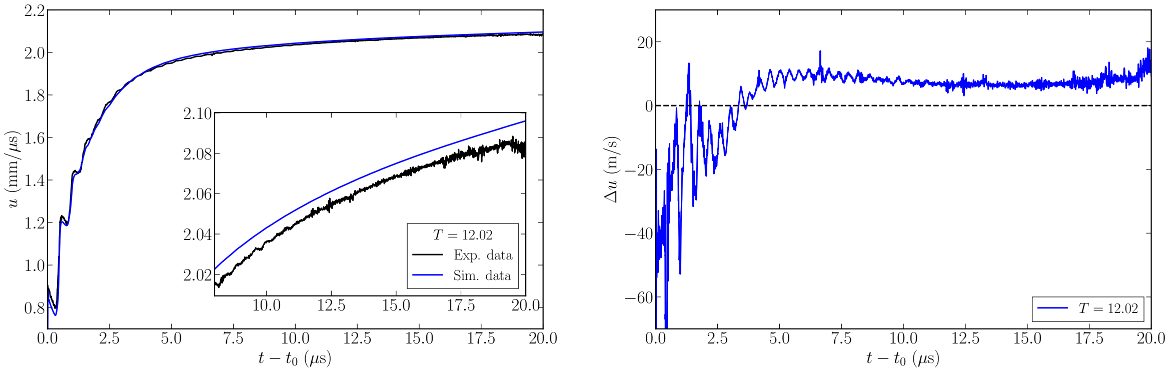

Figure 4: Comparison of the averaged experimental and the simulated motion of the outer surface of the Cu plates for the SLABEX test geometry. The simulations are based on the CYLEX-geometry calibrated PBX 9502 lot 008 JWL EOS model (Eqn. 1 and table 2). The figure on the right shows the corresponding difference Δu in the simulation and averaged experimental Cu plate velocity with time.

5 Summary

We have shown that the HE product JWL EOS for PBX 9502, populated by a hydrodynamic iteration technique in the CYLEX test geometry, has successfully passed the validation test of accurately describing the expanding Cu plate motion in a 2D SLABEX geometry. On-going work on this topic includes validation experiments and simulations on Cu confined two-dimensional arc geometries tests for PBX 9502 [19, 20].

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