Double shock experiments and reactive flow modeling on LX-17 to understand the reacted equation of state

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Abstract. Experimental data from measurements of the reacted state of an energetic material are desired to incorporate reacted states in modeling by computer codes. In a case such as LX-17 (92.5% TATB and 7.5% Kel-F by weight), where the time dependent kinetics of reaction is still not fully understood and the reacted state may evolve over time, this information becomes even more vital. Experiments were performed to measure the reacted state of LX-17 using a double shock method involving the use of two flyer materials (with known properties) mounted on the projectile that send an initial shock through the material close to or above the Chapman-Jouguet (CJ) state followed by a second shock at a higher magnitude into the detonated material. By measuring the parameters of the first and second shock waves, information on the reacted state can be obtained. The LX-17 detonation reaction zone profiles plus the arrival times and amplitudes of reflected shocks in LX-17 detonation reaction products were measured using Photonic Doppler Velocimetry (PDV) probes and an aluminum foil coated LiF window. A discussion of this work will include the experimental parameters, velocimetry profiles, data interpretation, reactive CHEETAH and Ignition and Growth modeling, as well as detail on possible future experiments.

1. Introduction
The insensitive high explosive (IHE) LX-17 (92.5% TATB, 7.5% Kel-F by weight) has slower reaction kinetics than conventional explosives as a result of the non-ideal behavior and presence of a 3-4 mm reaction zone length. The double shock technique was chosen to provide a method for measuring the reacted state and any observed kinetic effects at the rear sample/window interface using photonic Doppler velocimetry (PDV). The first shock detonates/reacts the energetic material and the second shock then travels through the reacted state. If the reaction in the initial shock is fast and complete, then the measured second shock (or re-shock) velocity should be equal to the isentropic (sound) wave speed in the material [1]. If the reaction is incomplete, interpretation would be necessary to correlate the second shock (or re-shock) wave speed to the true isentropic wave speed in the material. Previous research on reflected or overdriven experiments has been performed by a number of researchers [2-8]. The work here builds on a set of experiments performed using reflected shocks with manganin piezoresistive gauges to measure the initial and reflected shocks [9]. This paper will discuss the experimental setup used, PDV output velocities, comparison and interpretation of the data to modeling, and future work. The overall goal of this work is to measure the reacted equation of state, observe any kinetic time dependent effects, and compare to models for validation and improvement.
2. Experimental Procedure
Experiments were performed using the 2-stage gun at Lawrence Livermore National Laboratory (LLNL). Figure 1 shows a schematic of the experiment showing the polycarbonate sabot projectile with a 2 mm thick 304 stainless steel front flyer plate backed with 3 mm of tantalum. The target included a 1.5 mm thick 304 stainless steel buffer plate in contact with LX-17 (TATB based high explosive) that ranged from 3 to 8 mm thick and is backed by 10 mm of LiF as a window for the photonic Doppler Velocimetry (PDV) probes. A thin 12.7 µm foil of aluminum was placed between the LX-17 layer and the LiF window as a diffuse reflector material. A set of 6 time of arrival shorting pins was used to measure the impact arrival and subsequent tilt. In this experiment, the impact velocity was chosen to result in a pressure at or very near to the CJ pressure for the LX-17 sample. Therefore, with the LX-17 driven near CJ state and a supported shock then propagates through the sample. The velocity was recorded using measurements on the x-ray film as well as a series of laser photodiode velocity traps. An array of 4 PDV probes were used at the back of the target for observing the shock arrival times and particle velocity magnitudes, although in this paper only the center probes are reported and discussed for brevity.

![Figure 1](image_url)

**Figure 1.** A schematic of the double shock experiments performed using a 2-part flyer impacting a buffer plate in front of an LX-17 sample backed by a LiF window.

The Ignition and Growth reactive flow model [10] uses two Jones-Wilkins-Lee (JWL) equations of state, in the form:

\[
p = A e^{-k_{V}V} + B e^{-k_{2}V} + \omega C_{V} T / V \quad (1)
\]

where \( p \) is pressure, \( V \) is relative volume, \( T \) is temperature, \( \omega \) is the Gruneisen coefficient, \( C_{V} \) is the average heat capacity, and \( A, B, R_{1} \) and \( R_{2} \) are constants. The reaction rate equation is:

\[
dF / dt = I \left( \frac{1 - F}{\rho / \rho_{0} - 1 - a} \right) + \frac{G_{1}(1 - F)F^{d}p^{e}}{a_{e} - \varepsilon_{d}^{e} F_{1}} + \frac{G_{2}(1 - F)F^{c}p^{g}}{a_{c} - \varepsilon_{c}^{g} F_{1}} \quad (2)
\]

where \( F \) is the fraction reacted, \( t \) is time in \( \mu s \), \( \rho \) is the current density, \( \rho_{0} \) is the initial density, \( p \) is pressure in Mbars, and \( I, G_{1}, G_{2}, a, b, c, d, e, g, x, y, \) and \( z \) are constants.
The Cheetah detonation models are based on a multiscale approach to HE detonation modelling and is linked into the ALE3D model [11]. The Cheetah detonation models include more EOS features than the traditional Ignition and Growth model with a comparison of the details shown in table 1. Figure 2 shows an output of the species set mass fraction as a function of time. The current Cheetah detonation models are typically applied to steady detonation, and not normally used in shock initiation scenarios. The model also does not incorporate “fast kinetics,” although this is desired to implement in the near future.

Table 1. Comparison of modeling details for traditional reactive flow and the ALE3D/Cheetah detonation model.

| Detail            | Traditional reactive flow (ignition and growth) | ALE3D / Cheetah                  |
|-------------------|-------------------------------------------------|---------------------------------|
| Species set       | Reactant, product                               | > 30 chemical compounds        |
| Reaction rate     | Single reaction                                 | Multiple reaction               |
| Rate form         | Pressure dependent                              | Pressure or temperature dependent |
| Gas EOS           | JWL                                             | Exp-6 + dipole fluid model      |
| Solid EOS         | JWL                                             | Extended Murnaghan              |
| Number of phases  | 2                                                | > 3                             |

Figure 2. A plot of the species mass fraction as a function of time for the Cheetah detonation model.

3. Results and Discussion
The experimental details for the series of double shock experiments are shown in table 2 including the experiment number, date fired, impact velocity, and component dimensions. In the experiments, the thickness of the LX-17 samples was varied to provide some comparison information about the evolution of the wave as a function of distance travelled.
Table 2. Experimental details for the double shock experiments including component dimensions.

| Expt, date | Velocity (km/s) | Rear Flyer | Front Flyer | Buffer Plate | LX-17 | Reflector | LiF |
|------------|-----------------|------------|-------------|--------------|-------|-----------|-----|
| 4109, 4/18/12 | 3.511 km/s     | Ta, 3.022 mm | 304 SS, 2.019 mm | 304 SS, 1.508 mm | 19 mm Ø by 8.013 mm | 12.7 µm Al | 19 mm Ø by 10.016 mm |
| 4110, 4/20/12 | 3.518 km/s     | Ta, 3.018 mm | 304 SS, 2.020 mm | 304 SS, 1.509 mm | 19 mm Ø by 5.995 mm | 12.7 µm Al | 19 mm Ø by 10.078 mm |
| 4111, 4/24/12 | 3.916 km/s     | Ta, 3.016 mm | 304 SS, 2.018 mm | 304 SS, 1.495 mm | 19 mm Ø by 5.015 mm | 12.7 µm Al | 19 mm Ø by 10.031 mm |
| 4112, 4/26/12 | 3.737 km/s     | Ta, 3.020 mm | 304 SS, 2.023 mm | 304 SS, 1.496 mm | 19 mm Ø by 3.014 mm | 12.7 µm Al | 19 mm Ø by 10.028 mm |

Figures 3 and 4 display the center PDV probe signals for the set of experiments outlined in Table 2. Although only the center probes are shown, the center probes were compared to the probes on an outer perimeter with some slight probe-to-probe variations indicating 2-D effects (some due to tilt of impact) in the remaining probes. Further analysis of this data ongoing and will be included in a later publication. The experimental results are compared to the Ignition and Growth and Cheetah detonation modelling in order to gain an understanding of kinetic effects. The specific details of the modeling parameters used are not included here due to space limitations, but will also be included in a later publication with the additional analysis. As seen in figures 3 and 4, the shape of the 2nd arrival shock shows a more “rounded” front for all experiments that appears to indicate some additional reaction and maybe kinetic effects in LX-17. Neither of the models used currently have any “fast kinetics” built into them so it is unrealistic to expect a perfect match. However, the basic features in the experiments are reproduced in the comparison. In reviewing experiments 4109 and 4110 in figure 3, the initial shock and decay are seen in the experiment with the rounding of 2nd shock arrival seen in the experimental data, but not in the model results. The timing looks comparable to the models without an exact match of the experimental profile. For the slightly higher velocity experiments in figure 4, experiment 4111 shows the initial shock and decay in the experiment with rounding of 2nd shock and experiment 4112 shows a similar behavior although due to the thinner sample a “ring-up” is evident with an additional shock at later time. The comparison to the model again provides a general agreement without an exact match of profile. Additional experiments are in progress extending these experiments to lower and higher velocity regimes to obtain additional data to measure the extent of observing these features. The differences that are observed in model to experiment will guide future code development.
4. Summary and Future Work

The double shock method was used to measure the reacted equation of state in LX-17. These experiments built on previous work and utilized a PDV technique to measure the double shock with a lithium fluoride (LiF) window. Comparisons of the experimental data to Ignition and Growth and Cheetah Detonation models revealed that the main features matched reasonably well with some fine differences still needing to be resolved. Differences are thought to be a result of fast kinetics and will help drive future code development.

Future work on modeling is planned to include investigating 2-D effects as well as including more resolution of the experiment features (entire projectile, surrounding target holder, etc.) to validate using a simpler model and/or better match the small features. Future experiments are in progress using a similar target configuration with the 2-stage gun over a wider range of overdriven pressures with additional interest in heated/cooled environments.
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