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Experimental Determination of Chapman-Jouguet Pressure Using Disc Acceleration eXperiment (DAX) Data

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Abstract. The Disc Acceleration eXperiment (DAX) is, by now, a well-established small-scale detonation performance test that has shown a high degree of versatility. However, determination of Chapman-Jouguet (CJ, or detonation) pressure has proven challenging for less than ideal explosives applying the methods described in the seminal work of Lorenz et al. (*Propell. Explos. Pyrot.*, 40(1):95-108, 2015). In this study, two independent analysis techniques are presented to extract CJ pressure from DAX data. The first method relies on impedance matching and the compressible motion of the DAX witness disc. The second method uses previously developed one-dimensional equations of motion as well as an “effective mass” concept. Emphasis is placed on description of the methods rather than their application. Furthermore, hydrodynamic modeling is employed to highlight the physical phenomena underpinning the two techniques. It is shown that the latter method is preferred as it yields more accurate results and is applicable to ideal as well as non-ideal explosives.

Introduction

The Chapman-Jouguet (CJ) pressure (i.e., detonation pressure) is a characteristic property of chemical explosives that is fundamental to the understanding of detonation phenomena. It provides an important calibration point for detonation models (e.g., the ZND model¹⁻³) as well as for the equation of state (EOS) of detonation products.⁴ In addition, CJ pressure is an important measure when assessing the performance of a given explosive (e.g., through its correlation with brisance⁵), which is of relevance to practical design applications.

CJ pressure, however, is a challenging property to determine empirically to a satisfactory degree of accuracy. All available measurement techniques in-

fer the CJ pressure by performing observations in inert media placed in contact with explosives.⁵⁻¹³ Arguably, the most accurate of such techniques is that in which the free surface velocities of plates of different materials and/or thicknesses are measured.^{6-10,13} However, this approach is time intensive and costly; therefore, there is value in the development of simpler tests (e.g., [5, 11, 12]) to measure CJ pressure without detriment to accuracy.

Recently, Lorenz et al.^{14,15} developed a reduced-scale explosive material performance test: the Disc Acceleration eXperiment (DAX). The DAX stemmed from the need for a low-cost test requiring moderate amounts of material. The DAX is a rate stick that includes piezoelectric pins (to measure detonation velocity) and a thin metal witness

disc at the end of the stick. Once the stick is detonated, the disc is launched and its velocity is monitored via photonic Doppler velocimetry (PDV).¹⁶ Lorenz et al.¹⁵ demonstrated a technique to determine CJ pressure which relies on extrapolations based on features related to the initial velocity history of the DAX disc. For non-ideal explosives, however, such features may not be present, which render the results of this technique questionable.

On the basis of the discussion above, the work described herein presents methodologies (which extend and complement the study of Lorenz et al.¹⁵) for the determination of CJ pressure from DAX data. In the context of a DAX test, one can reasonably assume that the detonation is steady and one-dimensional. Under such conditions, the dynamic behavior of the DAX disc can be analyzed in two independent ways to yield CJ pressure. The methods are detailed and analyzed below using available data for LX-16,¹⁵ a plastic-bonded explosive containing pentaerythritol tetranitrate (PETN).

Approach

Reverberation Analysis Method

Figure 1 shows a DAX velocity-time profile of a 0.254 mm thick copper disc launched by the detonation of a 12.7 mm diameter and 152.4 mm long stick of LX-16 (96.5 wt% PETN in a VCTFE binder; initial density, $\rho_0 = 1.734 \text{ g/cm}^3$). The compressible motion of the disc is evidenced by the ringing oscillations (i.e., reverberations) in the velocity record. These reverberations are produced by shock wave interactions with the detonation products. Impedance matching^{17,18} (i.e., continuity of velocity and stress across interfaces) can be applied to obtain the conditions at the interface between the disc and the detonation products. In Fig. 1, each step change in velocity denotes a shock reflection at the free surface of the disc (i.e., even-numbered states in Fig. 1). The amplitude of this change can be used to estimate the particle velocity at the interface with the detonation products (i.e., odd-numbered states in Fig. 1):

$$u_{p,i} = \frac{1}{2} (u'_{p,i-1} + u_{p,i+1}) \quad i = 1, 3, 5, \dots \quad (1)$$

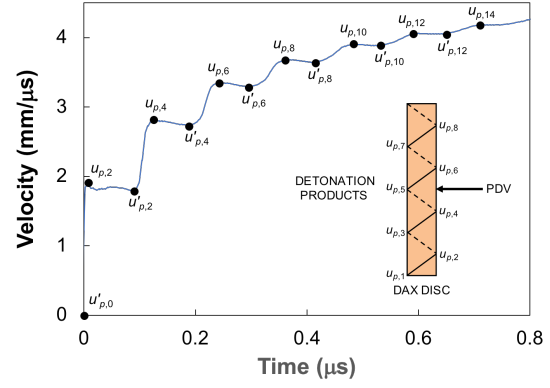


Fig. 1. DAX data for LX-16. The velocities needed for the evaluation of Eqn. 1 are noted. The inset shows an $x-t$ diagram of the shock reverberation process.

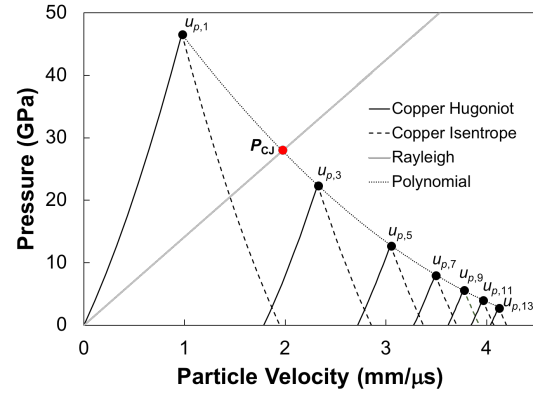


Fig. 2. Determination of CJ pressure. The particle velocities noted are obtained from Eqn. 1; the intersection of the Hugoniot and isentrope curves with the abscissa are the velocities (i.e., $u'_{p,i-1}$ and $u_{p,i+1}$ in Eqn. 1) recorded in the DAX test, see Fig. 1.

where $u'_{p,i-1}$ and $u_{p,i+1}$ denote, respectively, the “valleys” and “peaks” of the velocity record, see Fig. 1.

The DAX disc compresses and expands along its Hugoniot and isentrope, respectively. If one approximates the isentrope by the Hugoniot, the pressures at the interface can be calculated with the particle velocities obtained from Eqn. 1, see Fig. 2. In the present study, Hugoniot data for copper were

taken from Ref. 19. The pressure data in Fig. 2 can be fitted rather well by a second degree polynomial. Knowing that the CJ state must lie in a straight line^{8,9} of slope $\rho_0 D$ (where D is the detonation velocity), i.e., the Rayleigh line, its intersection with the fitted curve defines the CJ pressure, see Fig. 2. The CJ pressure derived for LX-16 using the method above is $P_{CJ} = 27.91 \pm 0.19$ GPa, where the uncertainty stems from the error in the coefficients of the polynomial fit. This value is approximately 8% lower than the 30.3 ± 0.4 GPa value determined by Lorenz et al.¹⁵

One-dimensional “Effective Mass” Method

If the detonation wave that impacts the metal disc in the DAX test is steady, planar, and one-dimensional, the terminal velocity reached by the disc can be described by the equations of Aziz et al.²⁰ for the motion of a piston under detonation loading. For a DAX experiment, the terminal velocity is determined by plotting the disc velocity in terms of scaled displacement, see Fig. 3. The scaled displacement is the time integral of the disc velocity normalized by the disc diameter, i.e., the diameter of the explosive. As shown in Fig. 3, the disc reaches an asymptotic/terminal velocity when it has moved a distance equivalent to one diameter. The equations of Aziz et al.²⁰ express the terminal velocity in terms of the detonation velocity, the polytropic gamma of the detonation gases, and a mass factor. In the DAX test, however, both the detonation and disc terminal velocities are known; therefore, the polytropic gamma, γ , can be solved for:

$$\gamma = \sqrt{8 \left[\frac{D(z-1)}{U(z+1)} \right]^2 + 1} \quad (2)$$

where U is the disc terminal velocity and z is the mass factor:

$$z = \sqrt{1 + \frac{32 C_{eff}}{27 M}} \quad (3)$$

where M is the mass of the DAX disc and C_{eff} is an effective charge mass acting onto the disc. This effective mass arises because of side losses, manifesting as rarefaction waves, that reduce the amount of explosive available to drive the DAX disc to a right circular cone behind the disc.

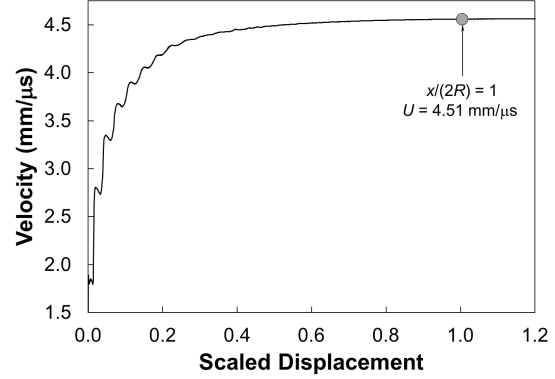


Fig. 3. Velocity data shown in Fig. 1 versus disc displacement (x) normalized by its diameter ($2R$). The terminal (i.e., asymptotic) velocity is noted.

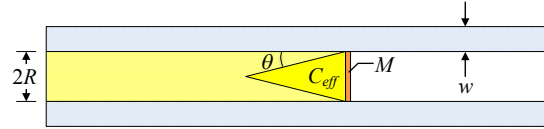


Fig. 4. Simple schematic of a DAX assembly showing the concept of effective mass. The discount angle, θ , and effective charge, C_{eff} , contributing to the acceleration of mass M are noted. The confinement (typically PMMA for DAX^{14,15}) of thickness w is also shown; R is the radius of the explosive.

Schematically, the effective mass concept is shown in Fig. 4. The angle, θ , that defines the effective mass depends on the mass of material confining the explosive:²¹

$$\theta = \frac{\pi}{6} \left[1 + 2 \frac{\rho_w}{\rho_0} \frac{w}{R} \left(2 + \frac{w}{R} \right) \right]^{-\frac{1}{2}} \quad (4)$$

where ρ_w is the density of the confining material, w is the wall thickness of the confinement, and R is the radius of the explosive. With Eqn. 4, then, the effective mass is:

$$C_{eff} = \rho_0 \frac{\pi R^3}{3 \tan \theta} \quad (5)$$

Finally, the CJ pressure is obtained with the polytropic gamma calculated from Eqn. 2:

$$P_{CJ} = \frac{\rho_0 D^2}{\gamma + 1} \quad (6)$$

For the LX-16 data considered here, Figs. 1 and 3, $D = 8.162 \text{ mm}/\mu\text{s}$, $U = 4.51 \text{ mm}/\mu\text{s}$, $M = 0.287 \text{ g}$, $R = 6.35 \text{ mm}$, $\rho_w = 1.182 \text{ g/cm}^3$ (PMMA), and $w = 6.35 \text{ mm}$. Application of Eqns. 2-6 yields $P_{\text{CJ}} = 30.7 \text{ GPa}$, in excellent agreement with the results of Lorenz et al.¹⁵

Discussion

The disparate results from the two methodologies described above warrant further examination. In this section, hydrodynamic modeling is used to gain further insights and provide physical arguments to explain the observed differences. All simulations discussed herein were performed with an in-house arbitrary Lagrangian-Eulerian code.²² The DAX geometry was treated as two-dimensional and axisymmetric. Adaptive mesh refinement was employed; the spatial resolution at the most refined level was approximately $35 \mu\text{m}$. This resolution was sufficient for the purposes of the present study.

Given that the reverberation method for extracting detonation pressure relies on the compressible “ring-up” motion exhibited by the disc (see Fig. 1), processes that may affect this motion need to be considered. One such process is the shock compression of the disc material, which is affected by its strength. Figure 5 shows DAX velocity curves simulated with and without the use of a constitutive model for the disc material; pressure and particle velocities (similar to Fig. 2) extracted from

these curves are also shown. In the simulations, the disc material was modeled with a Mie-Grüneisen EOS along with the Steinberg-Guinan constitutive model²³ (when used). The explosive was modeled via “programmed burn” using lighting time to propagate the detonation front and a compression based burn model (i.e., “beta burn”) with a JWL EOS for the detonation products of LX-16 taken from Lorenz et al.¹⁵

Note from Fig. 5 that in the absence of a constitutive model the amplitude of the reverberations increases along with the determined CJ pressure. The increase in this case is just over 3%, which does not fully account for the 8% underprediction noted above. This result indicates that there may be other phenomena that further compound the material strength effect shown in Fig. 5. Recently, Sutherland et al.²⁴ have shown, via hydrodynamic modeling, that possible voids (whether unfilled or filled with mineral oil or grease, as typically done experimentally) present between the explosive and the DAX disc can noticeably affect the reverberation process. The results of Sutherland et al.²⁴ were reproduced by the present authors and are not shown here for the sake of brevity. Finally, approximating the DAX disc isentrope by its Hugoniot (vide supra) introduces additional error,²⁵ on the order of 1%.

The one-dimensional effective mass methodology described in the previous section appears to provide accurate CJ pressure values, which may be

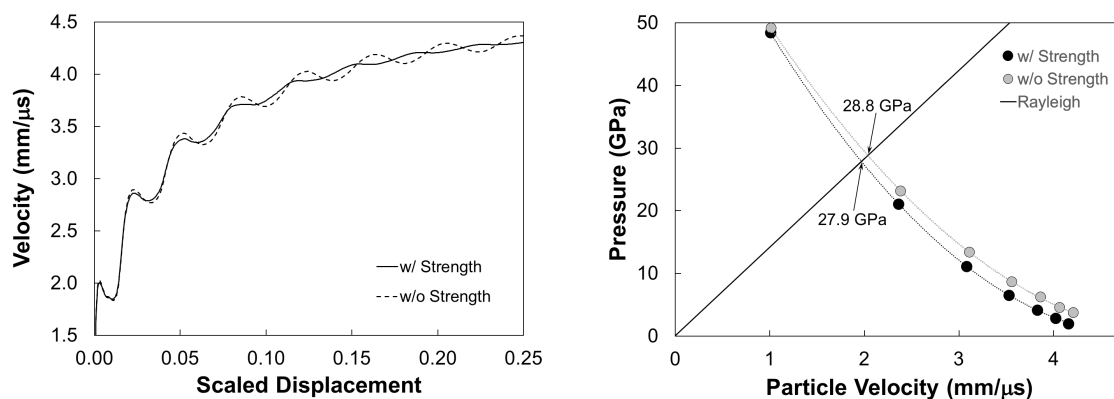


Fig. 5. (Left) Simulated DAX disc velocities, for the conditions of the data in Fig. 1, including or neglecting the strength of the disc material. (Right) Results of the reverberation method using the simulated disc velocities.

unexpected given the rather simplified (i.e., one dimensional) treatment of the problem. This method suggests that the asymptotic velocity of the DAX disc is governed by the CJ pressure as well as the geometry of the DAX. Furthermore, although not discussed herein, the one-dimensional effective mass method has been applied to ideal and non-ideal explosives with positive results. This observation is counterintuitive since it has been established¹⁴ that the DAX is sensitive to kinetic effects exhibited by non-ideal explosives.

To further investigate how detonation pressure and burn kinetics affect the DAX disc velocity, hydrodynamic modeling was applied to two explosive formulations widely varying in ideality. These explosives are PBX 9404 (94/3/3 wt% HMX/nitrocellulose/CEF) and LX-17

(92.5/7.5 wt% TATB/PCTFE). The modeling was performed as described above; however, the explosive programmed burn model was replaced by a JWL++²⁶ reactive flow model. This latter model consists of a Murnaghan²⁷ EOS for the unreacted explosive, a JWL EOS for the reacted explosive, a pressure mixer, and a pressure-dependent reaction rate. More details can be found in Refs. 14 and 26. All parameters needed for the simulations were taken from the study of Lorenz et al.¹⁴

The results of the reactive flow simulations are shown in Fig. 6. There is a difference in disc kinetic energy of approximately 40%, which correlates with the detonation energy of the explosives^{14,15} and shows the difference in their performance. Also in Fig. 6, the disc velocity sensitivities to CJ pressure and reaction rate can be found.

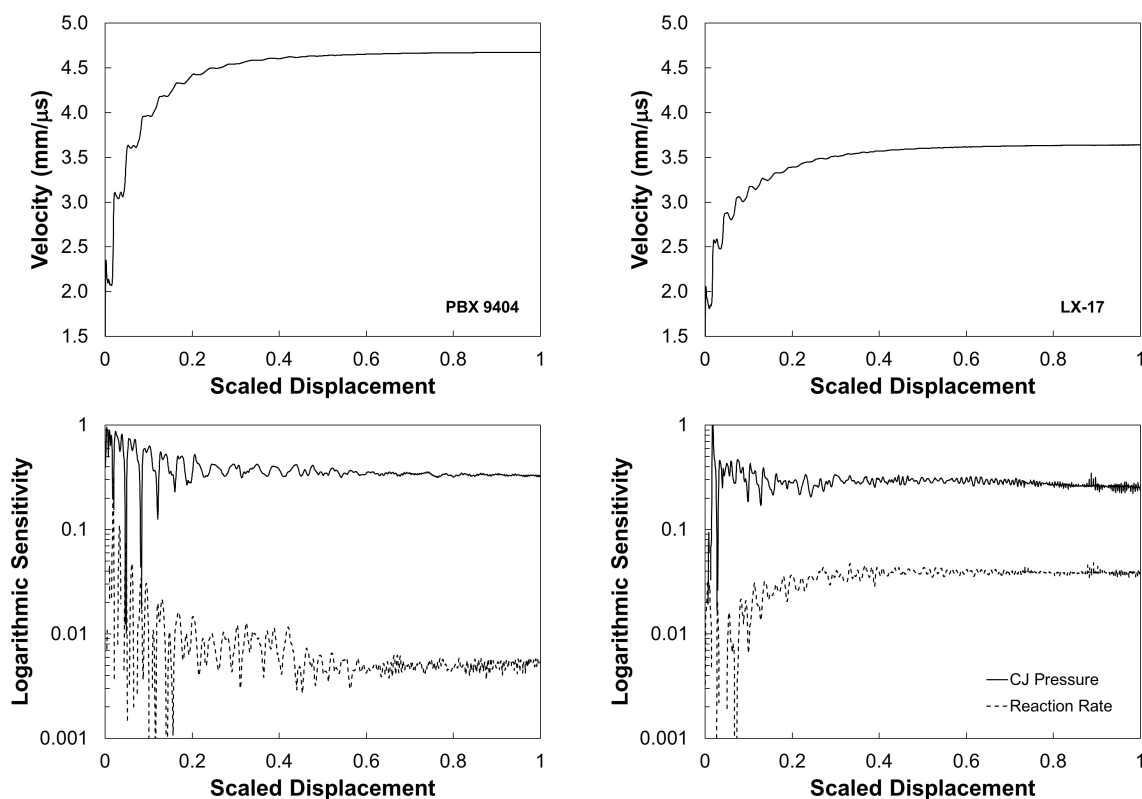


Fig. 6. Simulated DAX disc velocities (top row) and sensitivities to CJ pressure and reaction rate (bottom row) for PBX 9404 (left column) and LX-17 (right column). All simulations used a JWL++ reactive flow model with parameters from Ref. 14. The DAX geometry is identical to the LX-16 example of Figs. 1-5. Conditions - PBX 9404: $\rho_0 = 1.830 \text{ g/cm}^3$, $D = 8.80 \text{ mm}/\mu\text{s}$; LX-17: $\rho_0 = 1.903 \text{ g/cm}^3$, $D = 7.46 \text{ mm}/\mu\text{s}$.

These sensitivities were computed by comparing the base velocity values in Fig. 6 to those obtained by perturbing the CJ pressure and the reaction rate. When changing the CJ pressure, the JWL EOS was also modified to ensure its consistency with the new pressure as well as to maintain the same overall energy as the original JWL EOS. Note that the sensitivities shown in Fig. 6 are logarithmic, that is:

$$s = \frac{\partial(\ln y)}{\partial(\ln p)} = \frac{p}{y} \frac{\partial y}{\partial p} \quad (7)$$

where s is the sensitivity coefficient, y is the observable of interest (i.e., the disc velocity), and p is a given parameter (i.e., CJ pressure or reaction rate). Expressing the sensitivity in this manner ensures that the values are normalized so that direct comparison can take place.

Figure 6 shows that sensitivities are almost exclusively dominated by the CJ pressure. This is certainly the case in the asymptotic region (i.e., scaled displacement = 1), which is what is used in the one-dimensional effective mass method described above. For the less ideal explosive, LX-17, even though its sensitivity to reaction rate increases by approximately an order of magnitude over that of PBX 9404 (as expected), it is still an order of magnitude lower than its sensitivity to CJ pressure. It is also worth noting here that modeling shows that the effects of material strength and possible voids at the explosive/disc interface discussed above affect the asymptotic disc velocity by less than 2% so that the determined CJ pressure would vary by 1% or less. Therefore, the one-dimensional effective mass method appears to be a reliable way to determine CJ pressure.

Conclusion

Two independent methodologies have been presented to determine CJ pressure experimentally from DAX data. The first method, which relies on the dynamic reverberations exhibited by DAX discs, underestimates the CJ pressure. However, hydrodynamic modeling indicates that this is due to dissipative material effects as well as phenomena associated with experimental aspects (i.e., gaps/voids between the explosive and the DAX disc), which could be corrected for. Nonetheless, this methodology yields a useful lower bound on CJ pressure

without resorting to extrapolations¹⁵ that would be difficult to apply to data for less ideal explosives. Furthermore, this method can be applied to incomplete DAX records wherein the disc does not reach an asymptotic velocity.

On the other hand, the second method seems to provide accurate estimates of CJ pressure; this has been the case for a wide range of explosives (not presented herein) against which the present authors have tested this method. It has been shown through hydrodynamic modeling that the asymptotic velocity reached by the DAX disc, which is the basis of the methodology, is most sensitive to CJ pressure even for explosives that exhibit strong rate effects. Furthermore, the effects of material strength and experimental features do not strongly affect the asymptotic disc velocity. Therefore, this method appears to be sound and widely applicable.

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References

1. Zel'dovich, Ya. B., On the theory of the propagation of detonation in gaseous systems. *Zh. Eksp. Teor. Fiz.*, 10(5):542-568, 1940.
2. Neumann, J., Theory of Detonation Waves. Technical Report 549, Office of Scientific Research and Development, Washington, DC, 1942.
3. Döring, W., Über detonationsvorgang in gasen. *Ann. Phys.*, 43(6-7):421-436, 1943. doi:10.1002/andp.19434350605
4. Lee, E.L., Hornig, H.C., Kury, J.W., Adiabatic Expansion of High Explosive Detonation Products. Technical Report UCRL-50422, Lawrence Radiation Laboratory, Livermore, CA, 1968.
5. Pimbley, G.H., Bowman, A.L., Fox, W.P., Kershner, J.D., Mader, C.L., Urizar, M.J., Inves-

- tigating Explosive and Material Properties by Use of the Plate Dent Test. Technical Report LA-8591-MS, Los Alamos Scientific Laboratory, Los Alamos, NM, 1980.
6. Goranson, R.W., A Method for Determining Equations of State and Reaction Zones in Detonation of High Explosives, and its Application to Pentolite, Composition-B, Baratol, and TNT. Technical Report LA-487, Los Alamos Scientific Laboratory, Los Alamos, NM, 1946.
 7. Duff, R.E., Houston, E., Measurement of the Chapman-Jouguet pressure and reaction zone length in a detonating high explosive. *J. Chem. Phys.*, 23(7):1268-1273, 1955. doi:10.1063/1.1742255
 8. Deal, W.E., Measurement of Chapman-Jouguet pressure for explosives. *J. Chem. Phys.*, 27(3):796-800, 1957. doi:10.1063/1.1743831
 9. Deal, W.E., Measurement of reflected shock Hugoniot and isentrope for explosive reaction products. *Phys. Fluids*, 1(6):523-527, 1958. doi:10.1063/1.1724376
 10. Davis, W.C., Ramsay, J.B., Detonation pressures of PBX-9404, Composition B, PBX-9502 and nitromethane. *Proceedings of the Seventh Symposium (International) on Detonation*, Annapolis, MD, June 16-19, 1981, pp. 531-539.
 11. Cook, M.A., Keyes, R.T., Ursenbach, W.O., Measurements of detonation pressure. *J. Appl. Phys.*, 33(12):3413-3421, 1962. doi:10.1063/1.1702422
 12. Held, M., Determination of the Chapman-Jouguet pressure of a high explosive from one single test. *Defence Sci. J.*, 37(1):1-9, 1987. doi:10.14429/dsj.37.5886
 13. Pachman, J., Künzel, M., Němec, O., Majzlík, J., A comparison of methods for detonation pressure measurement. *Shock Waves*, 28(2):217-225, 2018. doi:10.1007/s00193-017-0761-5
 14. Lorenz, K.T., Souers, P.C., Lee, E.L., Chambers, R., Rapid, small-scale assessment of detonation performance using Disc Acceleration Experiments (DAX). *Proceedings of the Fifteenth Symposium (International) on Detonation*, San Francisco, CA, July 13-18, 2014, pp. 124-135.
 15. Lorenz, K.T., Lee, E.L., Chambers, R., A simple and rapid evaluation of explosive performance - the Disc Acceleration Experiment. *Propell. Explos. Pyrot.*, 40(1):95-108, 2015. doi:10.1002/prop.201400081
 16. Strand, O.T., Goosman, D.R., Martinez, C., Whitworth, T.L., Kuhlow, W.W., Compact system for high-speed velocimetry using heterodyne techniques. *Rev. Sci. Instrum.*, 77(8):083108, 2007. doi:10.1063/1.2336749
 17. Ager, T., Neel, C., Breaux, B., Vineski, C., Welle, E., Lambert, D., Chhabildas, L., Characterization of detonation products of RSI-007 explosive. *Shock Compression of Condensed Matter - 2011, AIP Conf. Proc.*, 1426:633-636, 2012. doi:10.1063/1.3686358
 18. Maines, W.R., Kittell, D.E., Hobbs, M.L., Combined mini-Cylex & disk acceleration tests in Type K copper. *Propell. Explos. Pyrot.*, 43(5):506-511, 2018. doi:10.1002/prop.201700296
 19. *LASL Shock Hugoniot Data*, Marsh, S.P. (ed.), University of California Press, Berkeley and Los Angeles, 1980.
 20. Aziz, A.K., Hurwitz, H., Sternberg, H.M., Energy transfer to a rigid piston under detonation loading. *Phys. Fluids* 4(3):380-384, 1961. doi:10.1063/1.1706337
 21. Benham, R.A., Analysis of the Motion of a Barrel-Tamped Explosively Propelled Plate. Technical Report SAND78-1127, Sandia Laboratories, Albuquerque, NM, 1978.
 22. DP Division Code Group, ARES Users Guide, Version 3.14. Lawrence Livermore National Laboratory, Livermore, CA, 2018. (Export Controlled)

23. Steinberg D., Cochran, S., Guinan, M., A constitutive model for metals applicable at high-strain rate. *J. Appl. Phys.* 51(3):1498-1504, 1980. doi:10.1063/1.327799
24. Sutherland, G., Sable, P., Borg, J., Simulations of disc acceleration experiments. *Shock Compression of Condensed Matter - 2017, AIP Conf. Proc.*, 1979:100040, 2018. doi:10.1063/1.5044912
25. Kerley, G.I., Calculation of Release Adiabats and Shock Impedance Matching. Report KTS08-1, Kerley Technical Services, Appomattox, VA, 2008.
26. Souers, P.C., Anderson, S., Mercer, J., McGuire, E., Vitello, P., JWL++: A simple reactive flow code package for detonation. *Propell. Explos. Pyrot.*, 25(2):54-58, 2000. doi:10.1002/(SICI)1521-4087(200004)25:2<54::AID-PREP54>3.0.CO;2-3
27. Murnaghan, F.D., The compressibility of media under extreme pressures. *P. Natl. Acad. Sci. USA*, 30(9):244-247, 1944. doi:10.1073/pnas.30.9.244