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INSENSITIVE HIGH EXPLOSIVE SHOCK-TO-DETONATION TRANSITION CRITERIA

Michael Gresshoff

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Michael Gresshoff

Lawrence Livermore National Laboratory, Livermore, CA 94550

Abstract. Insensitive high explosive (IHE) materials until recently have been qualified based on the results of eleven legacy experiments that input shock and thermal insults to candidate materials in a variety of configurations. Many of these qualification tests are obsolete or no longer conducted, ill-defined or ambiguous, and yield no data other than a material is screened to a standard or did or did not react. Presented here is criteria to qualify insensitive high explosives to shock that is clearly defined, may be used for model calibration, and results in data that may be used to assess margin to threshold. These new shock-to-detonation transition (SDT) criteria are based on one-dimensional shock pressures and durations into an explosive which are achieved using embedded gauge gas gun experiments. These shock criteria coupled with a new test to evaluate deflagration-to-detonation transition (DDT) and Bullet and Skid tests yields a more scientific and defendable definition of an IHE.

Introduction

The definition of an Insensitive High Explosive material, not to be confused with an Insensitive Munition (IM)[1], is found in the Department of Energy (DOE) Explosives Safety Standard[2] which states that "Some explosives substances, although mass detonating, are so insensitive that the probability of accidental initiation or transition from burning to detonation is negligible." Determination of whether a candidate explosive meets this definition has been accomplished by subjecting the explosive to eleven tests defined by the IHE standard. Passing all eleven tests and agreement by the DOE Explosives Safety Committee would result in approval of the candidate explosive as an IHE. To date, TATB (2,4,6-triamino-1,3,5-trinitrobenzene) and its formulations with Kel-F (poly (chloro-trifluoro-ethylene-co-vinylidene fluoride)) are the only approved IHEs.

The eleven IHE qualification tests were defined in the early 1980s and based on tests of the time used to screen and characterize energetic materials to various insults. Roughly forty years later, many of the eleven tests are no longer performed and obsolete (e.g., Susan Test) or are ill-defined (e.g., Card Gap Test and Detonation or Blasting Cap Test). Additionally, energetic material modeling and experimental capabilities have grown since adoption of these tests in the early 1980s. An opportunity exists to update the IHE qualification tests using a scientific and quantifiable assessment of the energetic material response. This new method would also yield data allowing for determination of margin to an insult and data characterizing the material versus a "Go / No Go" criterion or comparison to a poorly defined explosive standard such as Explosive D (ammonium picrate).

The fundamental characteristic of an IHE is its inability to undergo a deflagration-to-detonation transition (DDT), however, discussed in this paper is shock-to-detonation transition (SDT) threshold for IHEs. An IHE is required to undergo SDT as the function of the explosive is to detonate when intended to do so. A new threshold for SDT for an IHE should be sufficiently high such that the IHE will only detonate in an intended mode and not react in all other environments. Basing new criteria on environments that the explosive would be exposed to was considered, however, ultimately rejected due to environments constantly changing and having no bounds. Currently, the standard for assessing SDT is the use of a gas gun with embedded gauges in the energetic material to measure run-to-detonation distance as a function of input pressure[3,4,5] which is used to develop Pop Plots[6] and calibrate or validate reactive flow or unreacted equation-of-state (EOS) models.

Limitations of the existing Gap and Cap Test and a proposal for a new SDT criteria based on results of embedded gauge gas gun experiments on a candidate energetic material are discussed below. This new IHE SDT threshold was determined based on being consistent with the existing IHE shock threshold from the Card Gap Test with this threshold being equivalent to or less sensitive than Explosive D. The intention is that this new SDT criteria coupled with new tests for DDT, Skid Test, and Bullet Test would establish the qualification requirements for an IHE material replacing the existing eleven tests.

Legacy IHE Qualification Tests

Eleven qualification tests are defined in the DOE standard[2]. These tests are 1) Drop-Weight, 2) Friction, 3) Spark, 4) Ignition and Unconfined Burning, 5) Card Gap, 6) Detonation (Cap), 7) Cookoff, 8) Spigot, 9) Skid, 10) Susan, and 11) Bullet Impact. Reference 7 contains details of how the legacy tests are conducted. Of the eleven tests, two interrogate the shock response of a candidate IHE material: Card Gap and Cap Tests. The explosive response in the Spigot, Skid, Susan, and Bullet tests is complex due to these tests examining non-shock initiation (i.e., non-shock impact, friction, and/or shear of material leading to reaction or DDT).

Card Gap Test

The card gap test used to qualify TATB and its formulations with Kel-F 800 is defined in Reference 7 and is called the Pantex Modified NOL (Navy Ordnance Laboratory) Card Gap Test and is illustrated in Figure 1. Cellulose acetate cards, each 0.25-mm thick, attenuate the shock pressure out of the Pentolite (50% PETN, 50% TNT) donor and are stacked to find the threshold thickness of cards. Threshold is found with a 20-shot series and reported as a number of cards and a pressure. The pressure is assumed to be the pressure out of the cards which is consistent with how NOL and Naval Surface Warfare Center (NSWC) report results for the Large-Scale Gap Test (LSGT)[8]. An IHE candidate material is tested at least six times at the Explosive D 50% threshold thickness or less with no reactions. Detonation is considered a "well-defined crater-like dent" in a cold-rolled steel witness plate.

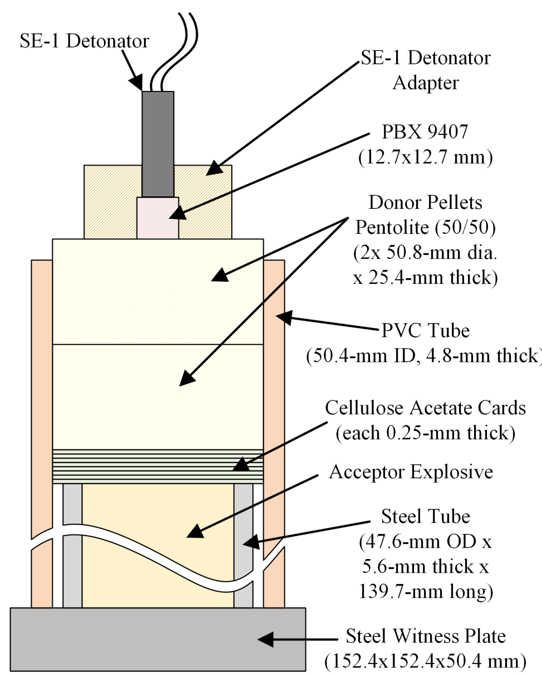

Figure 1. Pantex Modified NOL Card Gap Test. The NSWC LSGT is similar except uses PMMA (poly(methyl methacrylate)) cards, no PBX 9407

booster, and has a 1.59-mm air gap between the acceptor and the witness plate.

The gap test provides a metric (a quantity of cards) which allows for comparison to other explosives and a sense of margin to a threshold. However, the data is only relevant to the configuration of the test and cannot be used to predict the response of an explosive to shock in a different configuration. The shock is not one dimensional, is not sustained, and determines a threshold in a given configuration. Additionally, the IHE gap test requirement arbitrarily established Explosive D as the standard.

Figure 2 shows the result of a simulation of the Pantex Modified NOL Gap Test using Lawrence Livermore National Laboratory's multi-physics code ALE3D[9]. Shown is the curvature of the detonation front into the Explosive D acceptor. The shock input to the acceptor is not one-dimensional with the difference in shock arrival time from the centerline to the edge of the Explosive D being 311 ns along with the shock pressure not being constant or sustained as in a gun test as shown in Figure 8.

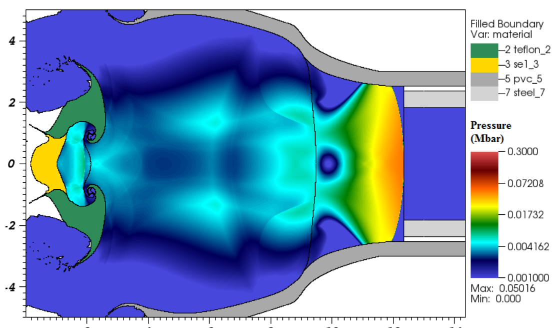

Figure 2. Two-dimensional axisymmetric ALE3D hydrocode simulation showing the front curvature at the cellulose acetate cards and Explosive D interface in the Pantex Modified NOL Gap Test. Contours are pressure in Mbar.

The Pantex test does not define Explosive D or Pentolite density and they are assumed to be 1.59 g/cc and 1.56 g/cc, respectively. No data was found characterizing the HE donor output or attenuators such as that found for NOL Card Gap Tests[10] and NSWC LSGT[8]. As will be shown later, this data will be used to calibrate a Pentolite model which will then be used to model the Pantex test and determine a shock-to-detonation transition threshold for an IHE consistent with the original standard and test.

Detonation (Blasting Cap) Test

The blasting cap test used to qualify TATB and its formulations with Kel-F 800 and the test defined currently in Reference 11 are different tests. The blasting cap test performed in the 1980s to qualify TATB is illustrated in Figure 3. The test was configured with a No. 8 blasting cap on the upper surface of a 5.1-cm diameter by 5.1-cm tall cardboard tube filled with explosive at ~110% of its bulk density. A detonation was defined as having occurred if the lead cylinder mushrooms 0.3 cm or more.

The current test defined in Reference 11 embeds the No. 8 blasting cap in the material being qualified versus on the top surface. Additionally, the current definition of a No. 8 blasting cap is not consistent with earlier definitions. The earliest reference found has No. 8 blasting caps having 1,511 mg of mercury fulminate/potassium perchlorate mixture in the "compressed" charge and 300 mg of mercury fulminate in the priming charge or roughly 2,000 mg of explosive[12,13]. Thermo-chemical code calculations[14] show the output detonation pressure of this compressed charge from the early 1900s would be 7.3 GPa versus ~27 GPa out of a modern No. 8 blasting cap[15]. With time, the No. 8 cap has changed and as defined currently is a minimum standard. Testing performed on current commercial No. 8 blasting caps and those used in the 1980s shows them to have significant differences in explosive output[16] with newer caps having greater output in terms of metal pushing energy measured with photonic Doppler velocimetry (PDV).

The blasting cap test is not an appropriate method for qualifying IHE materials because of the cap being ill-defined, variation in output of commercial No. 8 blasting caps, the test being performed in difference configurations over time, and that the test is on a bulk density material which is not relevant to assemblies with explosives pressed near their theoretical maximum density (TMD). The blasting cap test was developed to address transportation and storage safety and was used for IHE qualification because it was available at the time the IHE criteria were defined in the 1980s and TATB passed it.

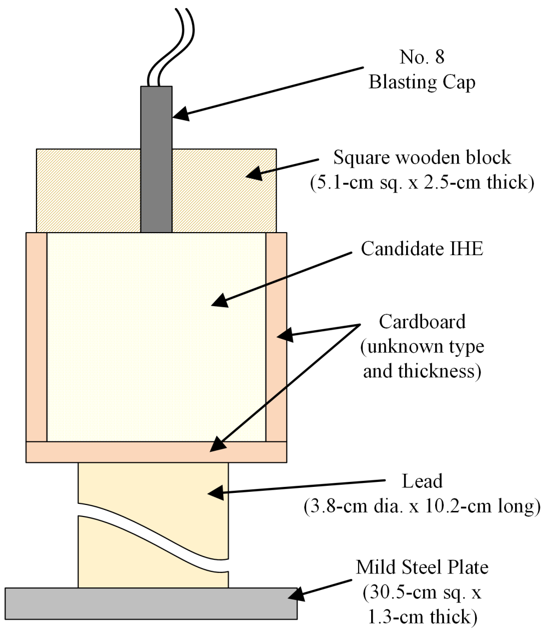

Figure 3. No.8 Blasting Cap Test as performed at Pantex to qualify TATB and its formulations with Kel-F 800 in the mid-1980s. This test differs from that currently defined in Reference 11.

Methodology and Results

Pursuing a threshold SDT criteria based on embedded gauge gas gun test results is preferred over modifying the legacy tests because of the issues with the gap and blasting cap tests discussed previously and the desire to develop modern criteria which yields data that has value in characterizing the material and establishing margin to threshold.

Initially, Pop Plot data for HMX- and TATB-based explosives was reviewed investigating a new SDT threshold. Setting the threshold half-way between HMX and TATB was considered, however, the goal was to not arbitrarily set a threshold and to investigate whether gap test results on Explosive D could be compared to data for HMX and TATB from run-to-detonation experiments such as embedded gauge gas gun tests. Numerous experimental series have been performed to determine the run-to-detonation distance on unconfined and ambient temperature (~20°C) TATB-based explosives LX-17-0 (92.5% dry-aminated TATB)[17,18], LX-17-1 (92.5% wet-aminated TATB)[19], PBX 9502 (95% TATB)[20,21,22,23], and Ultrafine TATB[24], and HMX-based explosives LX-04 (85% HMX)[25,26,27], LX-07-2 (90% HMX)[28,29], LX-10 (95% HMX)[28,29,30], and PBX 9501 (95% HMX)[28,31,32,33]. This data is shown in Figure 4.

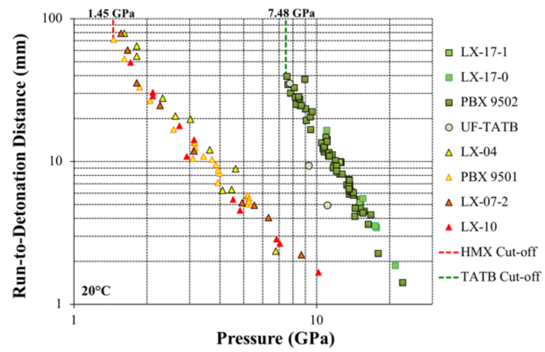

Figure 4. Pop Plot showing run-to-detonation distance of HMX- and TATB-based explosives.

To remain consistent with the legacy threshold, hydrodynamic analysis using ALE3D was performed on the Pantex gap test and NSWC LSGT with the goal of understanding the shock into Explosive D in the Pantex test and determining a shock pressure-duration threshold from it. Various Hugoniots were evaluated for the PMMA cards used in the Navy test[10,34,35,36,37,38,39,40] with the pressure-particle velocity relation shown in Figure 5. The variation in the PMMA Hugoniots below 30 GPa is small and subsequent simulations with PMMA cards used the material model and EOS from Tipton[39]. Sensitivity to variation in PMMA Hugoniots was also evaluated in the code and found to be negligible.

A JWL++ reactive flow model[41] for Pentolite was calibrated to Navy data[8] with the results shown in Figure 6. Pressure is accurately predicted by ALE3D at the interface between the PMMA cards and the high explosive acceptor. This Pentolite model is then used to model the Pantex results with cellulose acetate cards and Explosive D.

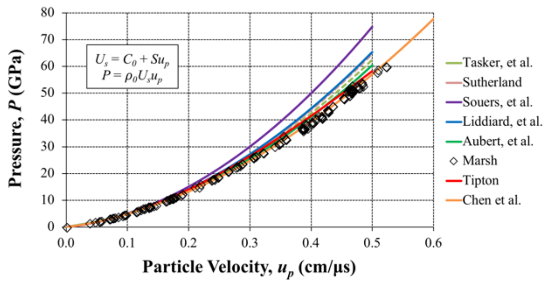

Figure 5. P-u_p relation for PMMA from multiple linear U_s-u_p Hugoniots. All, but one Hugoniot agrees well with others and data from Marsh below 30 GPa. PMMA $\rho_0 = 1.186$ g/cm^3.

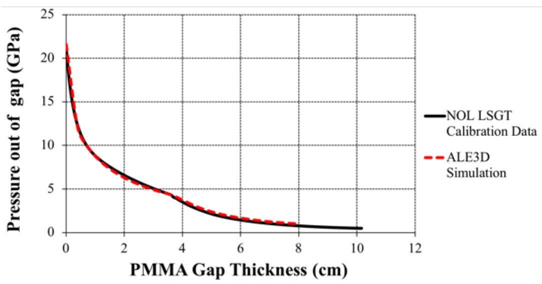

Figure 6. Pressure on centerline at card gap output from ALE3D simulation of NSWC LSGT compared to calibration (experimental) data. Pentolite JWL++ model was calibrated to NSWC data.

A Grüneisen EOS was calibrated to data from Marsh[38] for cellulose acetate cards used in the Pantex gap test. An unreacted EOS and material model was parameterized for Explosive D using a compaction model in ALE3D based on HMX compaction data[42] and EOS data collected using optical microscopy and interferometry on samples of Explosive D at LLNL[43]. Scanning electron microscopy of the Explosive D tested at LLNL is shown in Figure 7. The method used to measure the EOS of Explosive D is described in Reference 44. How well the HMX compaction data correlates to that for Explosive D is unknown as not data was found and insufficient quantity of Explosive D existed for testing.

Once the Pentolite, PMMA, cellulose acetate, and Explosive D models were calibrated, analysis of the Pantex test was performed into Explosive D along with analysis of the NSWC LSGT into HMX- and TATB-based explosives. Results for the Pantex gap test are that the threshold for Explosive D is 152.4 cellulose acetate cards (3.81 cm) with a pressure of 2.92 GPa, and for LX-17-0, 64 cellulose acetate cards (1.75 cm) with a pressure of 7.02 GPa[45]. Reference 8 states 165 PMMA cards (4.19 cm) at a pressure of 3.18 GPa for Explosive D and 200 PMMA cards (5.08 cm) for an explosive with a formulation similar to LX-10 (both 95% HMX) in the NSWC LSGT.

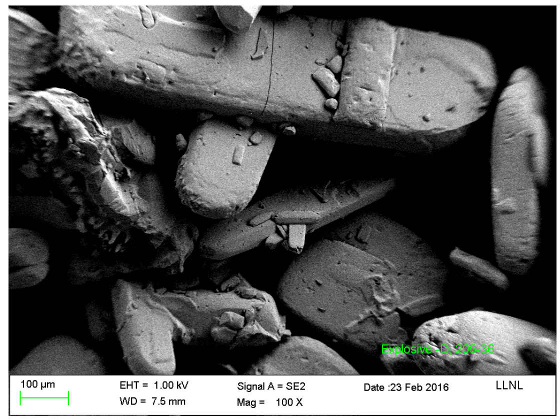

Figure 7. Scanning electron microscopy of Explosive D used to determine EOS. Median particle size of 236 μm was measured on a Micromeritics Saturn DigiSizer II 5205. It is unknown if this material is representative of what was tested in 1980s.

All simulations performed with ALE3D were two-dimensional axisymmetric on an orthogonal Eulerian mesh with an element size of 5 μm. Sensitivity to gaps between cards, overall attenuator thickness, and variation in Hugoniots were evaluated and a convergence study was performed with elements from 1 μm to 20 μm in size. Figure 8 shows results of a simulation of the Pantex gap test showing the difference in pressure and arrival time of the shock wave with a 3.81-cm card gap into 1.59 g/cc Explosive D.

In order to compare Pop Plot data in Figure 4 to simulations of the gap test, the Pop Plot run-to-detonation distance was scaled to initiation threshold shock duration using a method presented by James[46]. The results of this scaling are shown in Figure 9. Short-pulse shock initiation data for HMX-[47,48] and TATB-based[49] explosives was compared to pressure shock duration data from the Pop Plot. The time scaling factor for TATB-based explosives was approximated to be 0.31 which is equivalent to that given by James and 0.18 for HMX-based explosives, which is less than 0.23 given for PBX 9404 (94% HMX).

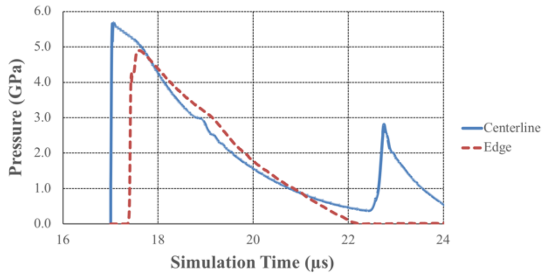

Figure 8. Pressure-time history predicted by ALE3D at the centerline and the edge of cellulose acetate card-Explosive D interface in the Pantex gap test.

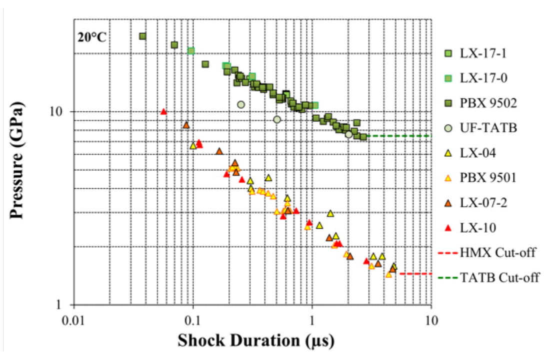

Figure 9. Pop Plot data converted into shock initiation data based on scaling the time to detonation into an initiation threshold shock duration. Scaling factors were chosen to be consistent with available short-pulse shock initiation data.

Figure 10 shows the results of ALE3D simulations of LX-17 (92.5% TATB) and Explosive D in the Pantex gap test and LX-10 (95% HMX) in the NSWC LSGT. The traces in the figure are the average pressure at the centerline (solid line) and edge of the explosive (dashed line) calculated using Equation 1.

$$P_{avg}(t) = \frac{1}{t_f - t_0} \int_{t_0}^{t_f} P(t)dt \qquad \text{(Eq. 1)}$$

Detonation of the explosive is assumed to occur once sufficient time at pressure is reached or when the average pressure-time trace intersects the scaled-to-initiation threshold Pop Plot data. The TATB-based explosives require longer shock duration for initiation than the HMX-based explosives which is consistent with short-pulse shock initiation data.

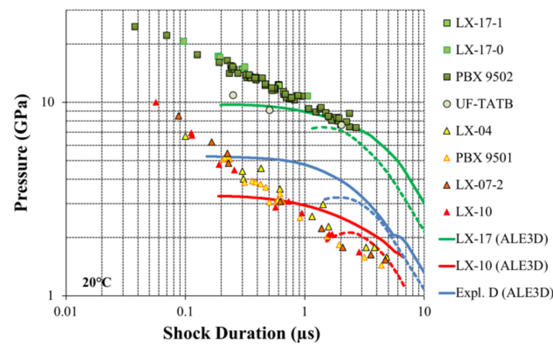

Figure 10. Results of ALE3D analysis on Pantex gap test with Explosive D and LX-17 and NSWC LSGT on LX-10. The solid lines are on the centerline of the explosive and the dashed lines are the pressure-time evolution at the edge of the explosive.

Figure 11 shows the same results presented in Figure 10 for Explosive D, but varying the gap thickness by 10%. Also shown are the proposed two points at which to evaluate candidate explosive materials for qualification as an IHE at ambient temperature. The two points are consistent with the legacy definition being defined by Explosive D based on simulation results.

In addition to ambient temperature criteria, an SDT criteria at elevated temperature to ensure the explosive does not sensitize beyond a reasonable level is prudent. Figure 12 presents Pop Plot data at elevated temperatures for LX-17[4,20,50], PBX 9502[20,50,51], PBX 9501[27,52], LX-04[4,26,53,54], and at ambient temperature for 1.72-g/cc PETN[27,55]. Defining an IHE SDT criteria without addressed the effect of temperature would be ignoring the safety conveyed by an IHE. Note in Figure 12 that TATB-based explosives at 250°C have a shock sensitivity equivalent to ambient temperature HMX-based explosives while HMX-based explosives at elevated temperature do not sensitize an equivalent amount to TATB.

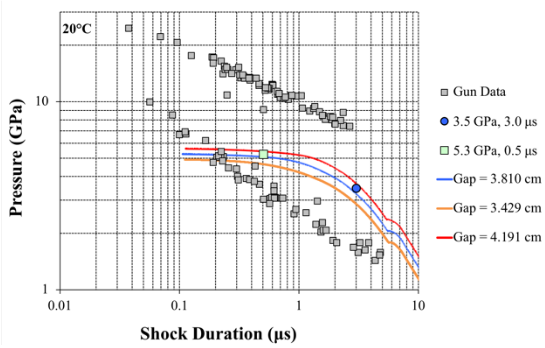

Figure 11. Ambient temperature SDT criteria for IHE. Also shown are the results of simulations varying the gap thickness by ±10%.

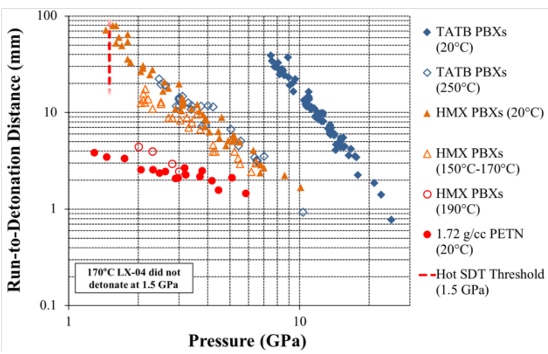

Figure 12. Pop Plot for elevated temperature HMX- and TATB-based explosives, and ambient temperature PETN. All test on unconfined explosive.

As shown in Figure 12, a pressure of 1.5 GPa is chosen as it bounds HMX data at elevated temperature. A shock duration of greater than or equal to 3.0 μs is chosen as it is of sufficient length and equivalent to the longer-pulse duration for the ambient test. The elevated temperature test is to be conducted at 10°C below the explosive's cook-off temperature. The cook-off temperature is defined as the temperature at which the material decomposes in the gun test configuration.

Discussion and Conclusions

The proposed new criteria for defining an IHE material with respect to SDT is no reaction at 20°C with pressure ≥3.5 GPa for a duration ≥3.0 μs, pressure ≥5.3 GPa for a duration of ≥0.5 μs, and at 10°C below cook-off temperature, pressure ≥1.5 GPa for a duration ≥3.0 μs. The shock pressures and durations above are for a one-dimensional, planar shock such that there is no effect from release waves from the edges of the explosive.

Arguments could be made that this new criteria is arbitrary, but it has been shown to be consistent to the existing criteria and has a basis beyond stating being half-way between HMX- and TATB-based explosives. It is fortuitous that the proposed threshold happens to fall roughly at this half-way point.

Adopting this new SDT criteria allows for the assessment of margin that a candidate energetic material has to the IHE shock threshold and provides data that can be used to parameterize high explosive models such as Ignition and Growth[56] and CREST[57, 58]. This new threshold also eliminates an ill-defined high explosive as a standard and provides a simple pressure and shock duration as the SDT requirement for an IHE. Embedded gauge gun tests using this criteria along with newly defined DDT, Bullet, and Skid tests provide a firm basis for defining an IHE.

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