LAWRENCE
LIVERMORE
NATIONAL
LABORATORY

LLNL-CONF-425266

Probabilistic Shock Threshold Criterion

Michael Gresshoff, Constantine A. Hrousis

May 14, 2010

14th International Detonation Symposium
Coeur d'Alene, Idaho, April 11-16, 2010

Disclaimer

This document was prepared as an account of work sponsored by an agency of the United States government. Neither the United States government nor Lawrence Livermore National Security, LLC, nor any of their employees makes any warranty, expressed or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States government or Lawrence Livermore National Security, LLC. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States government or Lawrence Livermore National Security, LLC, and shall not be used for advertising or product endorsement purposes.

Probabilistic Shock Threshold Criterion

Michael Gresshoff and Constantine A. Hrousis

Defense Technologies Engineering Division
Lawrence Livermore National Laboratory, Livermore, CA 94550

Abstract. The Probabilistic Shock Threshold Criterion (PSTC) Project at LLNL develops phenomenological criteria for estimating safety or performance margin on high explosive (HE) initiation in the shock initiation regime, creating tools for safety assessment and design of initiation systems and HE trains in general. Until recently, there has been little foundation for probabilistic assessment of HE initiation scenarios. This work attempts to use probabilistic information that is available from both historic and ongoing tests to develop a basis for such assessment. Current PSTC approaches start with the functional form of the James Initiation Criterion as a backbone, and generalize to include varying areas of initiation and provide a probabilistic response based on test data for 1.8 g/cc (Ultrafine) 1,3,5-triamino-2,4,6-trinitrobenzene (TATB) and LX-17 (92.5% TATB, 7.5% Kel-F 800 binder). Application of the PSTC methodology is presented investigating the safety and performance of a flying plate detonator and the margin of an Ultrafine TATB booster initiating LX-17.

Introduction

The Ignition and Growth (I&G) Reactive Flow Model is a constitutive kinetics model that can be calibrated to match 50% threshold sensitivity of high explosives (HE)[1]. Once tuned to a particular HE's response, I&G can be used to establish relative reactivity to a particular excitation and can provide insight into how an HE responds to a stimulus. It is not a kinematic model in that no geometry of burn is imposed (as in program burn models), but truly dynamic in that each finite element "decides" how much to react based on its local state. As such, I&G is a computationally expensive model to run, and when used in large engineering finite element models, I&G can be cost-prohibitive. In addition, I&G is tuned to an idealized 50% threshold and thus cannot directly provide the analyst with a sense of "margin to initiation".

In recent years, a simple approach has been proposed to get a sense of margin to initiation for high-speed impact problems. Hugh James[2] of the Atomic Weapons Establishment, UK, proposed an initiation criterion that built upon the previous critical energy fluence criterion of Walker and Wasley[3]. In addition to sufficient work performed on a surface (energy fluence), James identified that sufficient specific kinetic energy was simultaneously required. James showed that there existed a hyperbolically-shaped criterion in energy fluence versus specific kinetic energy space that separated initiation from non-initiation. Hrousis (LLNL) then proposed that one could define an initiation metric (J) based on the James Initiation Criterion, assume it to be randomly distributed due

to sample variability and experimental uncertainty, and quantify a margin against initiation (or non-initiation) by knowing the distance from the 50% threshold criterion coupled with the uncertainty in the threshold based on experiments. This approach, though significantly more crude than a simulation using a reactive flow model, provides some simple engineering insight on the likelihood of SDT (shock-to-detonation transition) in an HE subjected to high speed impact or excitation by a nearby donor charge. Combination of the James Initiation Criterion with an assumption about the initiation probabilistic distribution, and further amendments to account for diameter (2-D) effects results in a generalized "Probabilistic Shock Threshold Criterion" (PSTC) for future assessments.

Methodology

The James Initiation Criterion, as defined by James, is:

$$1 = \frac{E_c}{E} + \frac{\Sigma_c}{\Sigma} \tag{1}$$

$$E = p u_p \tau \tag{2}$$

$$\Sigma = \frac{u_p^2}{2} \tag{3}$$

The shock energy fluence or work done per unit area (E) was originally defined by Walker and Wasley for flat-topped shocks at a constant pressure, p, and particle velocity, u_p, over a finite time period, τ (Eq. 2). We suggest the following generalization for energy fluence:

$$E = \int p u_p dt \tag{4}$$

This form is intended to be applicable to general time-varying pressure histories, as would be expected from shock input from a donor explosive or other initiator (such as an exploding bridgewire), as well as for flat-topped shocks (e.g. from metal or plastic flyers). The specific kinetic energy (Σ) and the energy fluence using the integral representation are easily calculated for material points in a hydrodynamic analysis code. Both E_c and Σ_c are critical values for these energies and are material properties intrinsic to the HE, functions of its formulation and local density.

Though phenomenological, the concept of the James Initiation Criterion makes intuitive sense. Sufficient shock energy fluence (E) through a particular interface area is clearly needed for initiation, but it must occur before too much of it dissipates or transports away from the site of application. The local shock energy at the application site is captured by the Σ term, and if the needed energy fluence is not achieved before Σ dissipates, non-initiation is expected. It makes sense for shock initiation that there would exist a trade-off between magnitudes of E and Σ relative to their critical values, and thus the hyperbolic locus of points forming the initiation criterion. The cutoff concept introduced by Σ seems parallel to the run-distance required for detonation seen in Pop Plots, and the relationship between James Criterion and the Pop Plot has been explored by James[4].

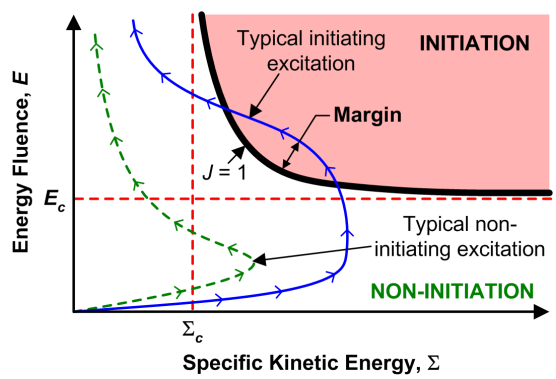

Figure 1. Concept of James Initiation Criterion. Shock input is translated into E vs. Σ space for material points in the explosive. If the explosive experiences states above and to the right of the James Criterion hyperbola, initiation is predicted.

Figure 1 illustrates the basic principle of the James Initiation Criterion: that when plotted in E vs. Σ space, initiating insults cause the HE to experience states above and to the right of the James Criterion hyperbola, while those that do not cause initiation remain below and to the left of the criterion. The principle suggests that marginal

initiations correspond to traces that barely touch the criterion, while robust initiating systems (in performance mode) delve greatly into the initiation regime and very safe non-initiating scenarios stay far away from crossing the criterion.

We suggest one way of quantifying HE excitation is to define a metric, the "James Number" (J), which defines hyperbolas that are parallel to the criterion, as follows:

$$\frac{1}{J} = \frac{E_c}{E} + \frac{\Sigma_c}{\Sigma} \tag{5}$$

We then identify J_{max}, the largest numerical value of J experienced in the HE, and assert that J_{max} is a viable metric for predicting initiation, in the following way:

$J_{max} = 1$ implies marginal initiation

$J_{max} > 1$ implies initiation (performance), with margin

$J_{max} < 1$ implies non-initiation (safety), with margin

This method appears to work best for simple, one-dimensional scenarios, where a large, non-diverging, planar insult is approaching a large slab of HE. The method begins to break down as the excited diameter of HE decreases and approaches the order of the critical diameter for that explosive. Decreasing excitation diameter causes the effective James Criterion to move up and to the right – it becomes harder to initiate. One way of capturing this effect is to quantify E_c and Σ_c as decreasing functions of excitation diameter (asymptotically approaching their 1-D values), though this form would make the material properties, E_c and Σ_c, subject to the geometry of the problem to be assessed.

We propose the following extension to the James Initiation Criterion to account for varying excitation diameters and call it the PSTC.

$$\frac{1}{\psi} = \frac{1}{J}\left[1 + \left(\frac{A_c}{A}\right)^k\right] \tag{6}$$

As the area, A, increases, the PSTC asymptotically approaches the one-dimensional form given as Equation 5 and as the area decreases, the threshold approaches infinity. Conveniently, the form of the PSTC (Eq. 6) results in the shock initiation threshold doubling in terms of James Number at the critical area, A_c (i.e. $J = 2$ at $A = A_c$).

Figure 2 illustrates the Probabilistic Shock Threshold Criterion. As the area decreases, the James Number required for initiation (the $\psi = 1$ line) increases. Where the one-dimensional criterion would suggest initiation of the HE with the maximum James Number greater than one as shown for the non-initiating excitation in Figure 2, the revised criterion shows that this case would not lead to initiation of the HE since it does not cross the shock initiation threshold or $\psi = 1$ line.

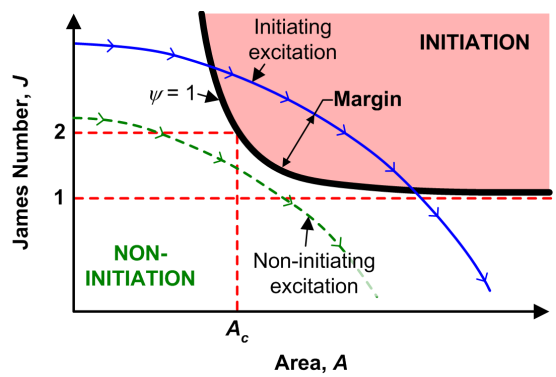

Figure 2. Illustration of the Probabilistic Shock Threshold Criterion. Shock input is translated into a maximum local James Number that is area-weight averaged and compared to the $\psi = 1$ threshold curve. The arrows on the excitations depict evolution over area (not time as in Figure 1) from the center of the shock insult.

Computational hydrodynamic analyses are used to determine the initiating and non-initiating traces shown in Figure 2. The energy fluence (Eq. 4) and specific kinetic energy (Eq. 3) are calculated from pressure and particle velocity time histories recorded at discrete locations (Lagrangian tracer particles) in the hydrodynamic computational domain. A rolling area-weighted average of the tracer particle maximum James Number is then calculated using Eq. 7 starting at the tracer particle located at the center of the

problem (axis of symmetry for two-dimensional calculations).

$$\bar{J} = \frac{J_{\max,i} A_i}{A} \tag{7}$$

The margin of initiation ($\psi - 1$) or non-initiation ($1 - \psi$) is then calculated as the trace distance from the PSTC threshold or $\psi = 1$ curve in J vs. A space with ψ calculated using Eq. 6.

Values for E_c, Σ_c, A_c, and k are determined from experimental data and I&G reactive flow model results. The experimental data used here to determine James Initiation Criterion and PSTC parameters for Ultrafine TATB (average particle size less than 10 μm and a surface area greater than 2.0 m^2/g) and LX-17 was collected during the late 1970s and early 1980s at LLNL using an electric gun[5] with the shock initiation threshold values based on this data having been reported by Weingart[6], Jackson[7], and Honodel[8]. The electric gun data consists of flyer material (typically Mylar), flyer thickness (0.051-1.27 mm) and diameter (1.6-25.4 mm), shot velocity into the HE, and whether or not the shot produced initiation. Impedance matching calculations are used to determine the experimental E and Σ based on a method presented by Cooper[9].

It is also desirable that the PSTC provide an engineering sense of the probability of initiation based on the maximum level of ψ experienced in the problem. The most important simplifying assumption to be made to accomplish this is the application of a probability distribution describing probability of initiation as a function of maximum ψ. Analysis of experimental data for flyer-impact initiation of 1.8 g/cc Ultrafine TATB yields not only the E_c, Σ_c, A_c, and k that place $\psi = 1$ at the 50% initiation point, but also σ_ψ, which is the best fitting one-sigma uncertainty in the $\psi = 1$ curve assuming normally distributed uncertainty. The σ_ψ parameter is most likely driven by experimental uncertainties, such as engineering tolerances, uncertainty and variability in flyer performance, etc. (epistemic uncertainty). It is also conceivable that it is affected by material-driven uncertainties as well, such as local variations in pressing density, variations in particle surface area, etc. (aleatory uncertainty). Both types of uncertainty are expected to exist in the designed application, as well as the experiment, and are assumed to be controlled to the same degree.

We initially fit the LX-17 initiation data assuming a normal distribution that proved overly conservative and we propose the use of a convolution of a normal and Pareto distribution. As will be shown, the corresponding probabilistic distribution curve for LX-17 does not appear to be symmetric (believed driven by initiation chemistry on the initiating side and experimental uncertainties on the non-initiating side). Equations 8 and 9 give the probability density functions (PDFs) for the normal distribution and the Pareto distribution, respectively. The PDF for the convolved Normal-Pareto distribution is given as Eq. 10 and the cumulative density function (CDF) as Eq. 11. The limits of integration on the equations are minus infinity and J or ψ, depending on whether the analysis is one-dimensional or uses the PSTC.

$$PDF_N(y) = \frac{1}{\sigma\sqrt{2\pi}} \exp\left(-\frac{(y-\mu)^2}{2\sigma^2} \right) \tag{8}$$

$$PDF_P(x) = \frac{a x_m^\alpha}{x^{\alpha+1}} \tag{9}$$

$$PDF_{NP}(x) = \int \{ PDF_N(y) \cdot PDF_P(x-y) \} dy \tag{10}$$

$$CDF_{NP}(x) = \int PDF_{NP}(x) dx \tag{11}$$

We are using I&G reactive flow models (which tend to independently reproduce the James Criterion threshold curve) to extend to other LX-17 excitation diameters for which we have limited experimental initiation data. This numerical data is analyzed along with the larger diameter experimental data to determine the PSTC parameters that place $\psi = 1$ at the 50% initiation point and the parameters for the probability density function. A maximum likelihood estimator, implemented using the solver function in Microsoft Excel, is used with a given probability distribution to fit the Ultrafine TATB

and LX-17 PSTC parameters to the experimental data.

We present hydrodynamic analysis using LLNL's multi-physics ALE3D[10] code to demonstrate uses of the PSTC methodology. We present analysis of barriers in a detonator to determine margin of initiation of the Ultrafine TATB acceptor HE. Figure 3 illustrates the detonator used by LLNL for various experiments including the barrier calculations discussed here. A 105-mg LX-16 (96.5% pentaerythritol tetranitrate (PETN), 3.5% FPC-461 binder) explosive pellet is initiated by a slapper (Kapton flyer). The LX-16 pellet detonates and drives a 0.127-mm thick aluminum flyer into the acceptor HE, which in this case is Ultrafine TATB. The detonator may also be configured with barriers for experiments investigating the level of safety provided.

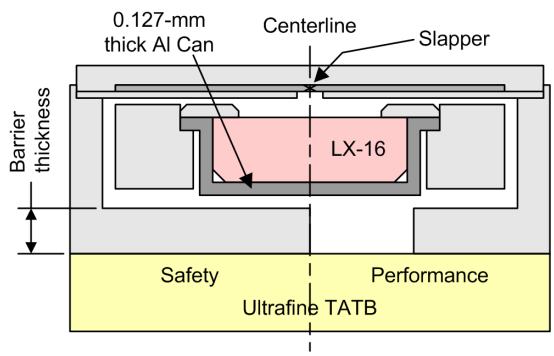

Figure 3. Detonator used for barrier and performance experiments. A slapper initiates an LX-16 pellet which drives a 0.127-mm thick aluminum flyer into the acceptor explosive. The left side of the centerline illustrates the safety mode with different thickness barriers and the right side of the centerline illustrates the performance mode.

We also present analysis using the PSTC methodology showing its application to experimental data without the use of reactive flow computational models. Fabry-Perot velocimetry data from Ultrafine TATB boosters with poly(methyl methacrylate) or PMMA windows yields particle velocity time histories from which pressure and energy fluence may be calculated with a Hugoniot for PMMA. Assuming energy fluence is constant, one may use the Hugoniot for LX-17 and calculate what the particle velocity would have been in the experiment if the surrounding material was LX-17. This is done by differentiating Eq. 4 with respect to time, setting $p = \rho_0 U_s u_p$, and then solving the cubic equation for u_p.

$$\left(\frac{\mathrm{d}E}{\mathrm{d}t}\right)_{\mathrm{PMMA}} = \left(\frac{\mathrm{d}E}{\mathrm{d}t}\right)_{\mathrm{LX\text{-}17}} = \rho_0 u_p^2 \left(C_0 + S u_p\right) \quad (12)$$

Once the equivalent LX-17 particle velocity is calculated, the pressure, James parameters (E and Σ), James Number, J, PSTC parameter (ψ), and probability of initiation may be calculated.

The input stimuli calculated in the analyses here (or experimentally determined) are assumed absolute for brevity. Figure 4 illustrates that this assumption can result in a non-conservative probability of initiation if not applied judiciously. Probability of shock initiation is influenced by both the uncertainty in the input stimulus and the location of the shock initiation threshold.

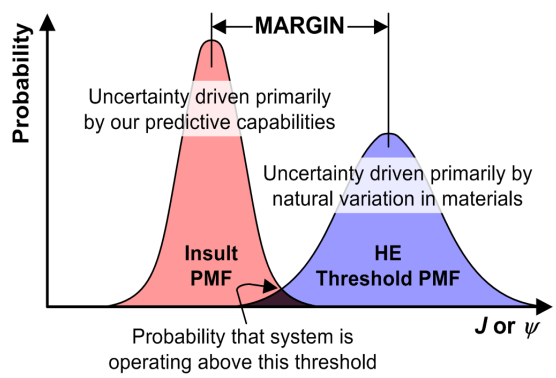

Figure 4. Illustration of the Probability Mass Functions (PMF) describing the location of the HE shock initiation threshold and a non-initiating insult or stimulus. The highest probability in the overlapping area is the probability that the insult is above the initiation threshold.

Results – 1.8 g/cc Ultrafine TATB

Figure 5 shows the electric gun data for 1.8 g/cc Ultrafine TATB and the PSTC threshold curve ($\psi = 1$) as a function of area. The threshold curve is determined by assuming the experimental

data are normally distributed. The 507 mm^2 data is from circular Mylar flyers with thicknesses of 0.051, 0.127, 0.254, 0.508, and 1.27 mm and the electric gun experimental data below 507 mm^2 is from Mylar flyers with a thickness of 0.254 mm only.

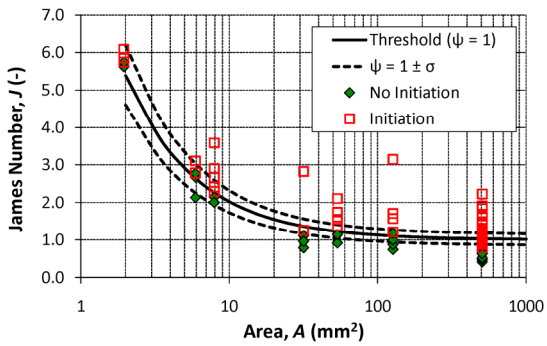

Figure 5. PSTC initiation threshold curve ($\psi = 1$) for 1.8 g/cc Ultrafine TATB. Electric gun data and the $\psi \pm 1\sigma$ curves are shown.

The PSTC parameters for 1.8 g/cc Ultrafine TATB assuming a normal distribution are:

$E_c = 0.210$ MJ/m^2
$\Sigma_c = 0.494$ MJ/kg
$A_c = 10.3$ mm^2 (Ø3.6 mm)
$k = 0.905$
$\mu_\psi = 1.00$
$\sigma_\psi = 0.147$

Figures 6 and 7 present the results of four separate hydrodynamic analyses performed using ALE3D. Energy fluence and specific kinetic energy density were calculated from pressure and particle velocity time histories from Lagrangian tracer particles spaced every 0.2 mm along the interface between the detonator and the Ultrafine TATB acceptor explosive starting at the axis of symmetry. The analyses presented in Figure 6 was performed using an Eulerian formulation at a mesh resolution of 500 zones per millimeter to investigate 0.051 and 0.102-mm thick steel barriers corresponding to the safety mode shown in Figure 3. Historical tests have shown that at ambient temperature, the 1.8 g/cc Ultrafine TATB initiates with a 0.051-mm thick barrier and the 0.102-mm thick barrier precludes initiation given detonation of the LX-16 pellet[11]. A high mesh resolution is required for the analyses to adequately resolve the particle velocity and pressure time histories used to calculate the maximum local James Number.

Using the PSTC probability distribution for Ultrafine TATB, the resulting margin is calculated as $(1 - \psi_{0.051}) = 0.03$ and $(1 - \psi_{0.102}) = 0.05$ with probabilities of initiation of $P_{0.051} = 0.43$ and $P_{0.102} = 0.37$.

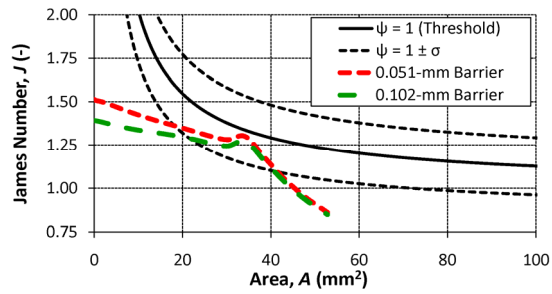

Figure 6. ALE3D calculations of 0.051-mm and 0.102-mm thick steel barriers with the detonator/barrier illustrated in Figure 3. PSTC predicts the experimentally determined threshold result within 1σ.

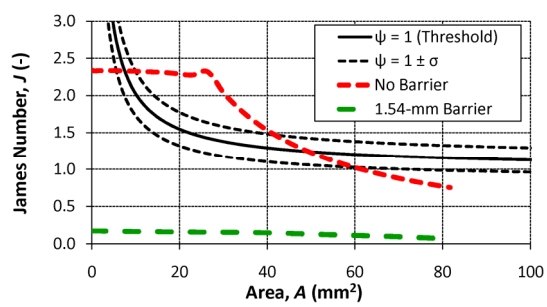

Figure 7. Performance and safety calculations of the detonator shown in Figure 3. The 1.54-mm thick steel barrier case (safety) falls multiple σ from the threshold and the performance case crosses the threshold curve indicating robust margin.

ALE3D analyses shown in Figure 7 give the margin on initiation for the "No Barrier" or performance case as $(\psi - 1) = 0.63$ with a probability of no initiation of $(1 - P) = 1\times10^{-5}$. The 1.54-mm thick barrier (safety) case's margin is $(1 - \psi) = 0.89$ with a probability of initiation of

$P_{1.54} = 8\times10^{-10}$. The methodology's uncertainty is in the location of the threshold and low probabilities of initiation or of no-initiation are essentially zero as ψ moves multiple standard deviations from the threshold line and far below the lowest "Go" or far above the highest "No-Go" experiment.

Results - LX-17 (92.5% TATB, 7.5% Kel-F 800)

Figure 8 shows the James Number calculated from electric gun data for flyers with 25.4 mm diameter and thicknesses ranging from 0.051 to 1.27 mm with constant sensitivity parameters, E_c and Σ_c. The data illustrates a dependence of the shock initiation threshold on the density of the HE and results in a large uncertainty in its location when using constant sensitivity parameters making margin assessment results overly conservative.

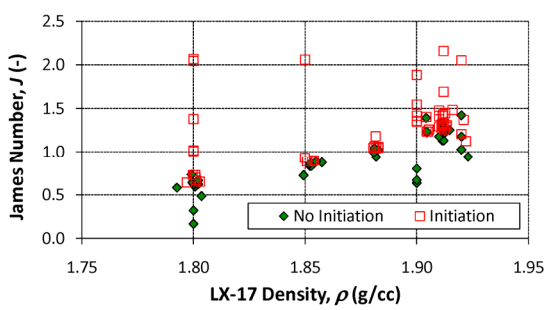

Figure 8. James Numbers for LX-17 electric gun experimental data showing the dependence of shock initiation threshold on HE density (E_c = 1.5 MJ/m^2 and Σ_c = 0.7 MJ/kg).

The PSTC parameters for LX-17 were calculated with E_c and Σ_c fitted as functions of density, which reduces the uncertainty in the location of the shock initiation threshold (J = 1 line) while assuming the data is governed by a convolved Normal-Pareto probability distribution. The one-dimensional James Criterion parameters for LX-17 calculated from experimental data as a function of density (assuming a second-order polynomial) are:

$$E_c(\rho) = 1.57 - 0.0279(\rho - \rho_0) - 6.96(\rho - \rho_0)^2 \quad (14)$$

$$\Sigma_c(\rho) = 1.85 + 21.3(\rho - \rho_0) + 60.4(\rho - \rho_0)^2 \quad (15)$$

These parameters are applicable for LX-17 with a density of 1.80 g/cc to 1.92 g/cc with the term ρ_0 equal to the theoretical maximum density of LX-17 (1.944 g/cc). Figure 9 illustrates how the uncertainty in the threshold has decreased with the threshold clearly about a James Number of one when using $E_c(\rho)$ and $\Sigma_c(\rho)$.

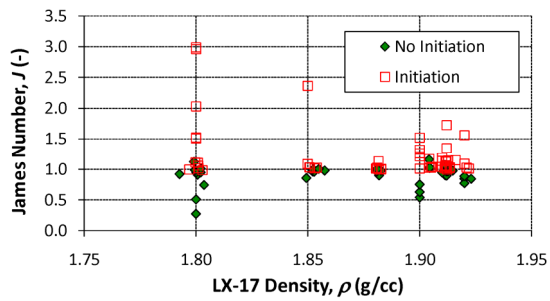

Figure 9. James Numbers for LX-17 electric gun experimental data with $E_c(\rho)$ and $\Sigma_c(\rho)$.

A normal distribution was initially used in fitting the PSTC parameters to the LX-17 experimental data and was found to be overly conservative. The convolved Normal-Pareto distribution, with the parameters below and shown in Figure 10, appears better suited to the problem at hand. As mentioned earlier, the Pareto distribution describes the chemistry in the response of the HE in that there is a hard limit below which the HE will not initiate. However, there is experimental error in determining that hard limit which is captured by the normal distribution. The convolution captures both the experimental error and the variation in the explosive properties. Figure 10 presents a "sanity check" of the probabilistic threshold analysis showing that the convolved Normal-Pareto distribution bounds the experimental data for both performance and safety calculations. The curve and experimental data points are not expected to overlay since they are determined using different methods, though they are related.

The convolved Normal-Pareto distribution (with the parameters below) is applicable to the one-dimensional James Criterion and is an estimation for the PSTC for LX-17 due to the lack of experimental initiation data other than reported 50% thresholds at flyer areas less than 507 mm^2.

Normal	Pareto
$\mu = 0.0$	$x_m = 0.964$
$\sigma = 0.0106$	$\alpha = 19.7$

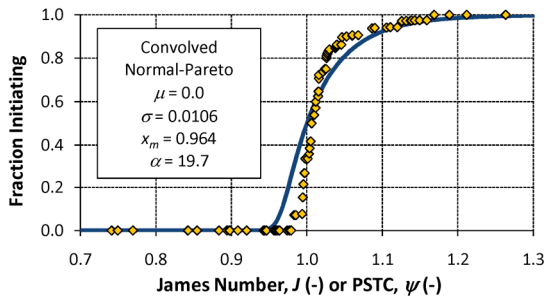

Figure 10. LX-17 experimental data illustrated as a fraction of the total data points that are initiating with the cumulative distribution function of the convolved Normal-Pareto distribution overlaid.

Experimental threshold series data at reduced diameters for LX-17 is not available, only reported 50% threshold values. To fit the PSTC area parameters for LX-17, reported threshold values[12] were used along with the electric gun experimental data with flyer diameters of 25.4 mm. LLNL's CALE[13] hydrodynamic code was used with the I&G reactive flow model to verify the reduced area threshold values. The same probability distribution governing the one-dimensional data is assumed to govern the PSTC since only threshold values are available and no threshold series data.

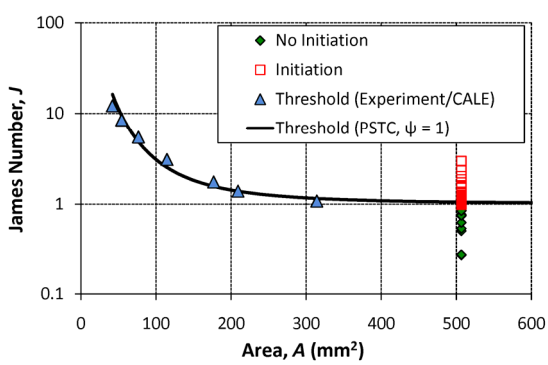

Figure 11. PSTC ($\psi = 1$) for LX-17. Electric gun data yields the one-dimensional threshold at 507 mm^2 and threshold values at reduced area are used to determine A_c and k.

Figure 11 shows the results of the fit to the threshold data with the one-dimensional $E_c(\rho)$ and $\Sigma_c(\rho)$ and the convolved Normal-Pareto distribution used to calculate the PSTC parameters for LX-17 accounting for area effect. It is interesting to note that the PSTC-calculated critical diameter of 13 mm is close to the traditional definition of the critical diameter, approximately 12 mm for LX-17[14].

$A_c = 138$ mm^2 (Ø13 mm)
$k = 2.30$

Analysis of Velocimetry Data

An application of the one-dimensional James sensitivity parameters for LX-17 is to investigate discrete points on the output of hemispherical booster charges. Figure 12 shows Fabry-Perot velocimetry data in E vs. Σ space collected by Druce *et al.*[15] at 7, 30, 60, 75 and 85 degrees off of the pole of a 38-mm diameter Ultrafine TATB booster initiated with the detonator shown in Figure 3. The measured particle velocity in the PMMA pressure transducers is adjusted using Eq. 12 to estimate what the particle velocity would have been had the Ultrafine TATB booster been surrounded with LX-17.

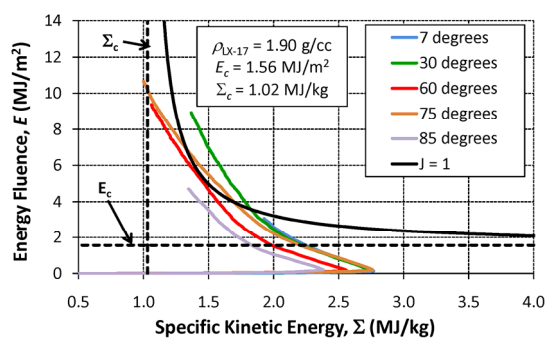

Figure 12. Fabry-Perot velocimetry data at different angles off of the pole (0° degrees) of a 38-mm diameter Ultrafine TATB booster into LX-17 (corrected from PMMA). The data was collected at ambient temperature.

Figure 12 shows that the 7 and 85 degree Fabry-Perot particle velocity traces are of insufficient length to determine a maximum James

Number or the maximum distance the excitation is from the threshold line. Additionally, plotting the velocimetry data in E vs. Σ space shows that a 38-mm diameter Ultrafine TATB booster has initiation margin at 30 and 75 degree with these excitations crossing the threshold line (J_{max} = 1.1 and 1.03, respectively), however, the 60 degree excitation is marginal (J_{max} = 0.99). Extrapolating the two Fabry-Perot records of insufficient length yields that 7 degrees would have $J_{max} > 1$ and $J_{max} < 1$ for 85 degrees.

Discussion

The LX-17 James sensitivity parameters (E_c and Σ_c) and the PSTC parameters accounting for area effects are a work-in-progress due to our current lack of threshold series data below a flyer area of 507 mm^2. The Fabry-Perot velocimetry data shown in Figure 12 suggests marginal initiation of LX-17 with a 38-mm diameter Ultrafine TATB booster where we know this to be a robust design at ambient temperature based on numerous experiments. This contradiction along with a PSTC analysis of Pantex Gap Test[16] data tabulated by Colville[17] for a range of LX-17 densities and analysis of LX-17 gun tests used to determine Pop Plots and corrected using a method proposed by James[4] suggest that the E_c term defined by Eq. 14 is correct, however, the Σ_c term (Eq. 15) may be reduced by a third. The reason for reducing the Σ_c term by up to a third is that the Σ_c term is largely defined by only two flyer data points. The reduction of Σ_c by a third is an approximation given the data we currently have and further experiments, especially with thicker, slower flyers, are required for the method presented here to calculate Σ_c with higher confidence.

Conclusions

The James shock initiation criterion and the PSTC have been shown to be useful tools to predict shock initiation and provide a probability of initiation. However, the PSTC is not a tool to predict HE performance such as with a reactive flow model in a hydrodynamic code. It is an engineering analysis methodology used to estimate the likelihood of an explosive to initiate given a specific shock input, whether that input excitation is determined experimentally, computationally, or analytically.

The James Criterion and the current PSTC both assume a non-divergent shock wave into an acceptor explosive. The PSTC builds upon the James Criterion defining margin (ψ) from the 50% initiation threshold while accounting for critical diameter effects. The current form of the PSTC does not account for shock divergence resulting in margin of initiation being over-estimated and margin of non-initiation being under-estimated (i.e., J and ψ are both over-estimated). Therefore, the current PSTC is conservative for safety assessments, but not for the calculation of performance margin. Addition of a divergence term to Eq. 6 is a focus of future work.

Our current work focuses on developing experiments to efficiently refine our calculated threshold in James and PSTC space for LX-17 and to better quantify the uncertainties in those thresholds. Other current work focuses on incorporating pressure history measurements via PDV (Photonic Doppler Velocimetry) into future initiation system performance measurements and to develop a PSTC parameter set for the explosives LX-10 (95% HMX, 5% Viton-A binder) and LX-16 based on data collected by May[18] and Tarver[19]. Future efforts will investigate broadening the problems to which the PSTC may be applied by adding or modifying terms to account for divergence and temperature effects to the shock initiation threshold.

Acknowledgements

The authors wish to thank Jeffrey D. Hagerty, Ronald S. Lee, George E. Overturf III, William McLean, Chadd M. May, and Ronald D. Streit for support. Thanks also to Hugh James, James F. McCarrick and John S. Christensen for multiple valuable conversations and peer review.

This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under contract DE-AC52-07NA27344.

References

[1] Tarver, C.M., Halquist, J.O., and Erickson, L.M., "Modeling Short Pulse Duration Shock Initiation of Solid Explosives" *Proceedings of the 8th International Detonation Symposium*, pp. 951-961, Albuquerque, NM, July 1985.

[2] James, H.R., "An Extension to the Critical Energy Criterion Used to Predict Shock Initiation Thresholds" *Propellants, Explosives, Pyrotechnics*, Vol. 21, pp. 8-13, 1996.

[3] Walker, F.E., and Wasley, R.J., "Critical Energy for Shock Initiation of Heterogeneous Explosives" *Explosivstoffe*, Vol. 17(1), pp. 9-13, 1969.

[4] James, H.R., "Links between Macroscopic Behaviour and Explosive Morphology in Shock to Detonation Transitions" *Proceedings of the 13th International Detonation Symposium*, pp. 952-961, Norfolk, VA, July 2006.

[5] Chau, H.H., Dittbenner, G., Hofer, W.W., Honodel, C.A., Steinberg, D.J., Stroud, J.R., and Weingart, R.C., "Electric Gun: A Versatile Tool for High-Pressure Shock-Wave Research" *Review of Scientific Instruments*, Vol. 51(12), pp. 1676-1681, 1980.

[6] Weingart, R.C., Lee, R.S., Jackson, R.K., and Parker, N.L., "Acceleration of Thin Flyers by Exploding Metal Foils: Application to Initiation Studies" *Proceedings of the 6th Symposium (International) on Detonation*, pp. 653-663, San Diego, CA, August 1976.

[7] Jackson R.K., Green, L.G., Barlett, R.H., Hofer, W.W., Kramer, P.E., Lee, R.S., Nidick, E.J., Shaw, L.L., and Weingart, R.C., "Initiation and Detonation Characteristics of TATB" *Proceedings of the 6th Symposium (International) on Detonation,* pp. 755-765, San Diego, CA, August 1976.

[8] Honodel, C.A., Humphrey, J.R., and Weingart, R.C., "Shock Initiation of TATB Formulations" *Proceedings of the 7th Symposium (International) on Detonation*, pp. 425-434, Annapolis, MD, June 1981.

[9] Cooper, P.W., "Rarefaction Waves", in *Explosives Engineering*, pp. 232-241, Wiley-VCH, Inc., New York, 1996.

[10] Nichols, A.L., "Users Manual for ALE3D: An Arbitrary Lagrange/Eulerian 2D and 3D Code System" Lawrence Livermore National Laboratory Report UCRL-SM-404490, 2009.

[11] Cheng, J., Cowan, M., and Davis, R.W, "Performance Margins of Booster Barriers" presented to the 24th Annual Joint Fireset Conference, 1999.

[12] Weingart, R.C. and Lee, R.S., "Initiation Studies of TATB-Based High Explosives" Lawrence Livermore National Laboratory Report UCID-20120, pp. 20, July 1984.

[13] Tipton, R., Managan, R., and Amala, P., "CALE Users Manual" Lawrence Livermore National Laboratory, July 2009.

[14] Tran, T.D., Tarver, C.M, Maienschein, J., Lewis, P., Moss, M., Lee, R.S., and Roeske, F., "Characterization of Detonation Wave Propagation in LX-17 near the Critical Diameter" *Proceedings of the 12th International Detonation Symposium*, pp. 684-692, San Diego, CA, August 2002.

[15] Druce, R.L., Roeske, F., Souers, P.C., Tarver, C.M., Chow, C.T.S., Lee, R.S., McGuire, E.M., Overturf, G.E., Vitello, P.A., "Propagation of Axially Symmetric Detonation Waves" *Proceedings of the 12th International Detonation Symposium*, pp. 675-683, San Diego, CA, August 2002.

[16] Tarver, C.M., "Modeling Shock Initiation and Detonation Divergence Tests on TATB-Based Explosives" *Propellants, Explosives, Pyrotechnics*, Vol. 15(4), pp. 132-142, 1990.

[17] Colville, J.C., "LX-17 Test Data" Mason & Hanger-Silas Mason Co., Inc. – Pantex Plant, pp. 23, 1990.

[18] May, C.M., and Tarver, C.M., "Modeling Short Pulse Duration Initiation of LX-16 and LX-10 Charges" *16th APS Topical Conference on Shock Compression of Condensed Matter*, Vol. 54(8), Nashville, TN, June-July 2009.

[19] Tarver, C.M., and May, C.M., "Short Pulse Shock Initiation Experiments and Modeling on LX-16, LX-10, and Ultrafine TATB" *Proceedings of the 14th International Detonation Symposium*, Coeur d'Alene, ID, April 2010 (in press).