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Characterization of Physical Processes During Thin-Pulse Initiation of Energetic Materials

David Damm and Evan Dudley

Sandia National Laboratories*
Explosives Technologies Group

PO Box 5800 MS1452
Albuquerque, NM, 87185-1452, USA
(505) 844-1247 (phone)
(505) 844-5924 (fax)
dldamm@sandia.gov

Eric Welle
Initiation Science and Technology Group
Air Force Research Laboratory, Munitions Directorate
Eglin AFB, FL

Abstract

Here we report on experimental and modeling efforts to characterize the effects of flyer diameter and thickness on thin-pulse initiation of fine-grained hexanitrostilbene (HNS). Photonic Doppler Velocimetry (PDV) measurements at threshold firing conditions over a range of input shock conditions provide the James Criterion parameters for thin-pulse initiation of HNS. The primary parameters reported here include spot size, shock amplitude and thickness. In addition to the experimental studies, hydrocode simulations of flyer impact and SDT response of the explosive material are being developed to improve our qualitative understanding of these processes. Upon flyer impact, the run up to detonation is simulated by a reactive burn model which predicts the local extent of reaction and couples the additional energy into the shock front. Although our preliminary results indicate qualitative agreement between the model and experimental data, the limits of the predictive capability of this modeling approach are of particular interest and will be quantified.

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Introduction

Processes that occur during the initiation of energetic materials when subjected the thin or short pulses has been of interest to the community for some time[1]. For the purpose of this discussion, we define a thin pulse as a shock imparted into the explosive material that does not have sufficient spatial/temporal thickness to support the entire initiation process to the point where a reaction wave that is only affected by curvature is propagating. Experimental and modeling efforts to characterize the effects of flyer diameter and thickness on thin-pulse initiation of fine-grained hexanitrostilbene (HNS) are in progress and the preliminary results are reported here. Photonic Doppler Velocimetry (PDV) measurements of flyer velocity at threshold firing conditions provide the James Criterion parameters[2] for thin-pulse initiation of HNS. In the James initiation (or trigger) model, critical values of energy fluence and specific energy must be exceeded for the explosive to undergo a shock to detonation transition (SDT). In addition to the experimental studies, hydrocode simulations of flyer impact and SDT response of the explosive material are being developed both to aid in design and to improve our qualitative understanding of these processes. Upon flyer impact, the run up to detonation is simulated by a reactive burn model which predicts the local extent of reaction and couples the additional energy into the shock front. Although the pressure-based phenomenological burn models show qualitative agreement with experimental data, the predictive capability of this modeling approach is of limited accuracy.

Experimental Results

Experiments have been conducted to determine the initiation threshold of fine grained HNS as a function of spot size and flyer thickness. The parameter levels were defined to specifically probe the thin-pulse initiation regime. The range of thicknesses evaluated overlaps well-documented experiments conducted by others[3,4] and extends into thicknesses that approach the practical limitations of the dielectric under evaluation. The data presented here represents combinations of three spot sizes (flyer diameters) and five flyer thicknesses. Bridge thickness and material, barrel length, and explosive density were held constant. At the time of this writing, the experimental matrix has not been completed but sufficient data has been collected to warrant discussion of the method and results to date and provide a substantial data set for use in the modeling discussion that follows.

The goal of the test series is to evaluate the thin-pulse initiation threshold of fine grained HNS in terms of the initiation criterion developed by James as an extension to the Walker and Wasley[5] critical energy criterion for shock initiation of heterogeneous explosives. The James criterion threshold curve can be determined from Equation 1 where critical values of energy per unit area (E_C) and specific kinetic energy (Σ_C) must be exceeded for the explosive to detonate.

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

Determination of the critical values for this set of experiments first required the determination of the firing voltage corresponding to the 50% threshold of initiation for each configuration using the Neyer method. Once the threshold firing conditions were established, direct measurement of flyer velocities at the threshold firing conditions were made. A Photonic Doppler velocimetry (PDV) system was used to collect velocity data from multiple shots for each configuration. Figure 1 is a schematic of that system where the reader should note that the balancing is done via the use of inline optical power monitor/attenuators which is similar to systems previous reported[6] .

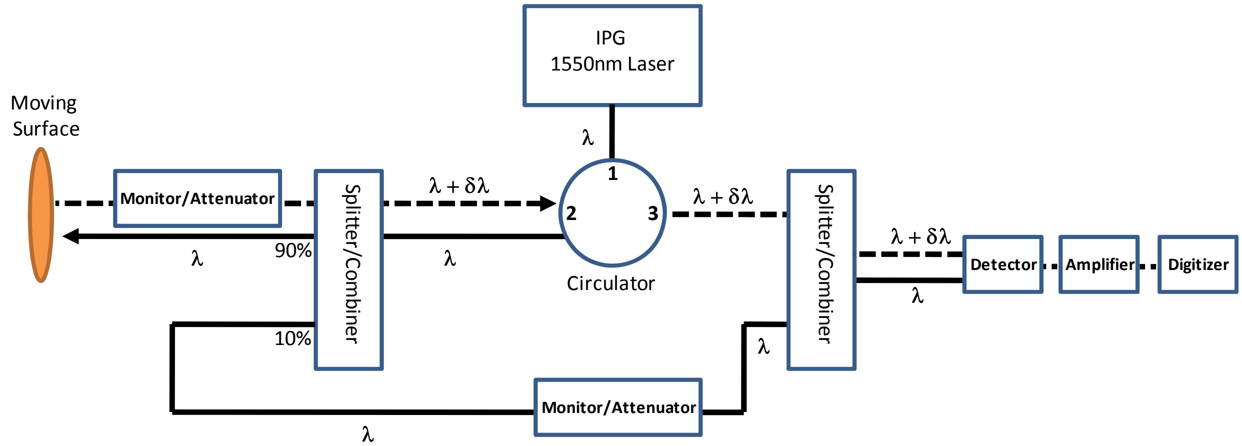
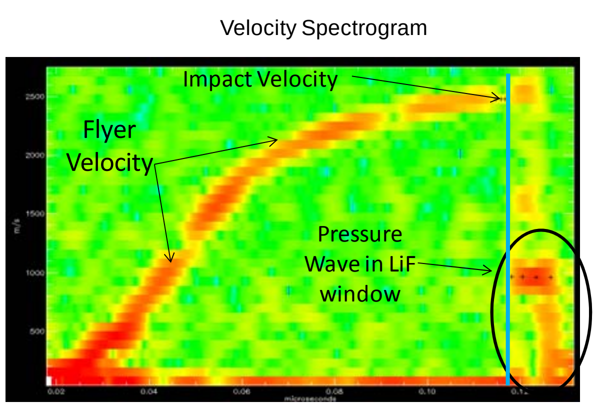


Figure 1. Schematic of the balance PDV system.

In each PDV test, the explosive column was replaced with a <100> oriented lithium fluoride window which allowed measurement of the flyer velocity history as well as the particle velocity and pulse duration upon impact with the window. A fast fourier transform (FFT) analysis was conducted on the raw data to obtain the FFT spectrum similar to that shown in Figure 2 using pTool analysis software[7] . The flyer velocity history is then extracted from the spectrum using pTool's velocity extraction function. Due to the shortest time durations of the shock pulses driven into the lithium fluoride widows being on the order of several nanoseconds, a zero crossing method was used to determine frequency (velocity) and duration using the raw time domain data. Window corrections were conducted using data reported by Jensen et al[8] .



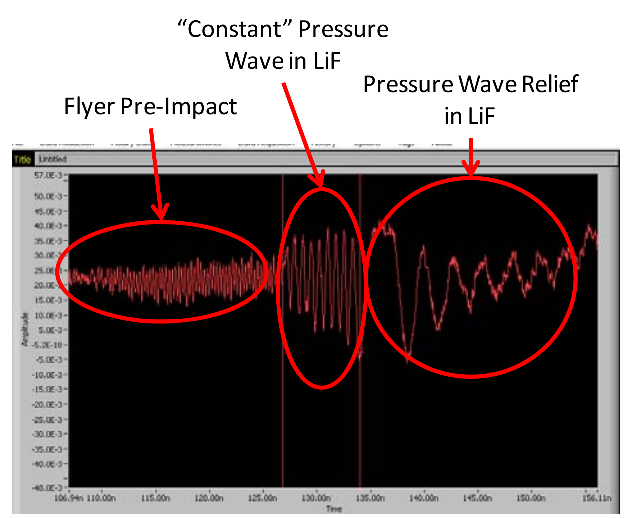


Figure 2. Sample FFT spectrum from PDV experiments showing flyer transit and impact with LiF window.

Once the threshold flyer velocity was obtained, the impact conditions in the HNS pressing were calculated using the un-reacted Hugoniot parameters reported by Goveas et al[9]. Using the calculated pressure (P), particle velocity (u_p) and pulse duration (τ), the energy per unit area (E) and specific kinetic energy (Σ) resulting from each test was calculated using equations 2 and 3.

$$E = P u_p \tau$$

$$\Sigma = \frac{1}{2} u_p^2$$

For the purposes of the present analysis, the constant pulse duration, τ, was taken as twice the shock transit time in the flyer following impact. This approximation was in good agreement with the constant pressure pulse data collected in the PDV experiments. Plotting the results as energy fluence vs. specific kinetic energy and fitting to equation 1 produces the James initiation criterion curve for thin-pulse initiation of fine-grained HNS given in Figure 3.

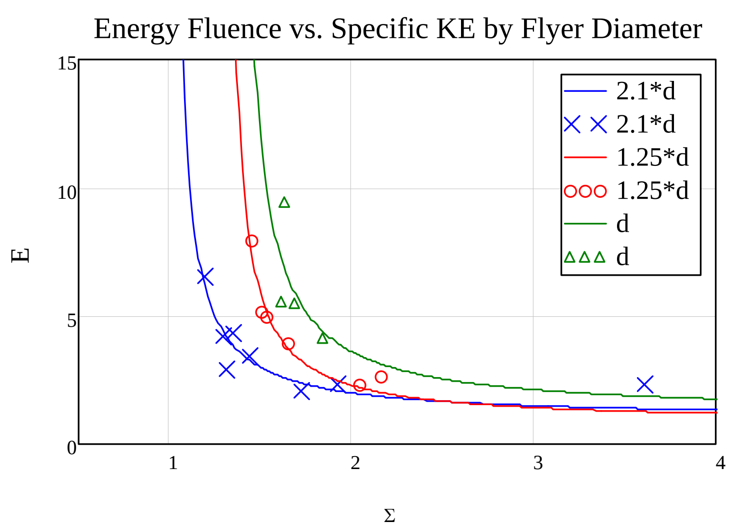


Figure 3. James criterion curve for thin-pulse initiation of fine-grained HNS for three flyer diameters. Data is scaled to critical E and Σ parameters for 2.1*d case.

Realizing the initiation process is a volumetric one, it is not surprising to see a shift in the initiation curve as a function of spot size as shown in Figure 3. Also, it is evident that E_c does not appear to change as a function of spot size. As spot size decreases, edge effects become more significant and as a result the initiation threshold tends to increase. It is clear that 1-dimensional assumptions have limited applicability in this range of flyer parameters. This limitation will be explored in the modeling section of this paper. The results are plotted as flyer velocity vs. normalized flyer thickness in Figure 4 for the three diameters.

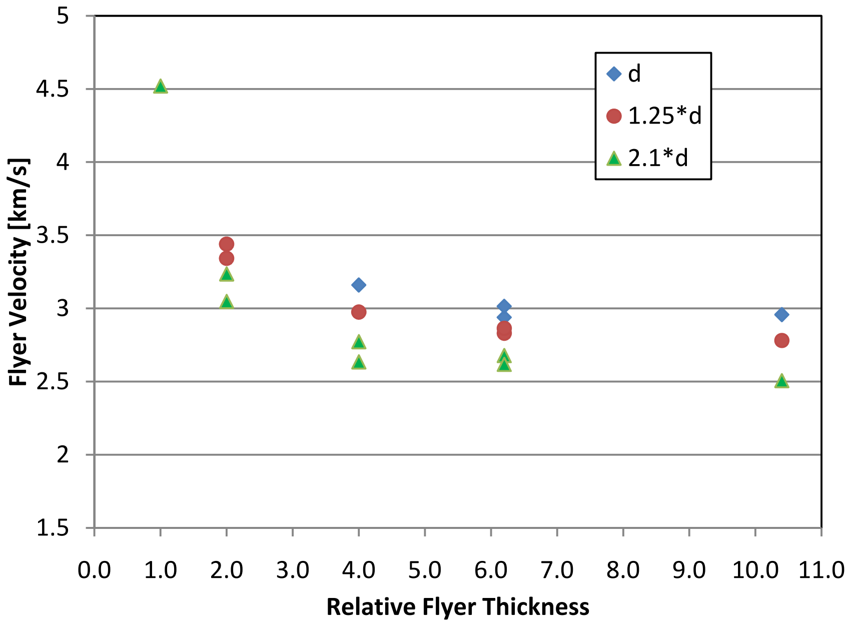


Figure 4. Flyer velocity vs. flyer thickness for three flyer diameters.

Modeling Approach

The History Variable Reactive Burn (HVRB) model, implemented in CTH, is commonly used for shock to detonation (SDT) and detonation transfer calculations. The HVRB model calculates the extent of reaction, λ:

$$\lambda = 1 - (1 - \phi^M / X)^X$$

which depends on the growth of the pressure-time integral, ϕ, which has the form:

$$\phi = \int_0^t \left(\frac{P - P_i}{P_R}\right)^Z dt$$

The parameters, M, X, Z, P_i, and P_R, are constants which are found by fitting the calculation to empirical data.

The standard procedure for calibrating the HVRB model parameters is to adjust P_R and the exponent Z to obtain agreement with pop-plot data[10]. Increasing or decreasing P_R shifts the calculated pop-plot to the right or left, respectively. Increasing or decreasing Z either increases or decreases the slope of the calculated line, respectively. Table 1 lists the values of the parameters that were used to obtain the fit shown in Figure 5. The data is from Kipp, et al[3] for a material of particle size, density, and specific surface area similar to that used in the experiments described above. The values of parameters M, X, and Pi, are default values that are assigned when no additional information is available. The porous density was set to 1.6 gm/cc with a crush pressure of 1.43 GPa[3].

Table 1. HVRB model parameters.

Parameter [units]	Value (HVRB 1)	Value (HVRB 2)
M	1.5	1.0
X	1.0	2.0
P_i [dynes/cm^2]	0.5e10	2.0e10
P_R [dynes/ cm^2]	4.25e10	3.3e10
Z	3.55	3.3

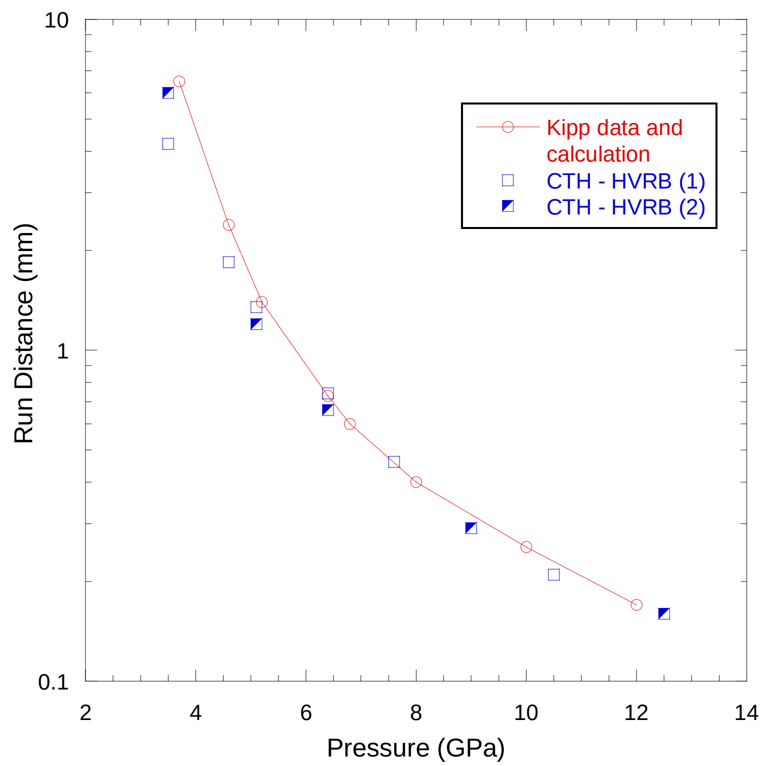


Figure 5. Pop-plot data[3] and HVRB run distance calculations for HNS.

Taking a closer look at the parameters, we observe the following:

- The term P_i is the threshold pressure for initiation[10]. It is by default assigned a value of 0.5 GPa based on the results of a published study in which the authors looked for evidence of chemical reactions (in propellants and plastic bonded explosives) induced by shock waves that were below the threshold for SDT[11]. It is questionable whether a true SDT model should be expected to consider sub-SDT pressures in a physically meaningful fashion. (Recently, a damage-induced reaction model was developed[12] to predict the response of energetic materials in the non-shock (or sub-SDT) pressure regime.) Therefore, it is reasonable to increase the value of P_i to near the minimum pressure at which SDT is reliably achieved.
- The parameter *X* controls the rate of completion of the reaction. $X < 1$ causes a very rapid (almost instantaneous) transition to detonation, once sufficient pressure (and extent of reaction) is reached. $X > 1$ slightly dampens this effect as the extent of reaction approaches completion.

- The parameter *M* controls the time delay behind the shock front for reaction to occur. For *M* =1, the reaction occurs near the shock front. For *M* >1, the reaction occurs behind the front. Kipp[3] noted that fine-grained HNS displays characteristics associated with homogeneous explosives (i.e. a superdetonation wave that overtakes the shock front). This implies that the reactions build up behind the shock front and *M* >1 is appropriate. However, Kipp also notes that at very high impact pressures (thin flyers), this behavior has not been observed (i.e. the behavior looks heterogeneous). The default value for HNS is *M* =1.5, but in our second HVRB model we have set *M* =1 to force the reactions to occur near the shock front. This does not imply that reactions occur instantaneously! The extent of reaction, ϕ, still depends on growth of the integral of pressure over time.

Without additional data, such as embedded pressure gage data[13] or cut-back experiments, we can only make an educated guess about the correct values of these parameters. On-going experimental efforts include cut-back studies to quantify the reaction growth process such that a more precise evaluation of reactive flow models can occur. The values for the second HVRB model are summarized in Table 1. Interestingly, both models fit the pop-plot fairly well (see Figure 5) despite the fact that they both use very different sets of parameters. Unfortunately, neither model is able to predict the correct threshold velocity for initiation by very thin flyers (see Figure 6). It is unclear whether or not there exists a single set of parameters that will result in an HVRB model which both fits the pop-plot *and* accurately predicts threshold velocities. If that set of model parameters exists, the best chance of finding it is to first calibrate the model to data which records the details of the growth of reaction and run-up/transition to detonation.

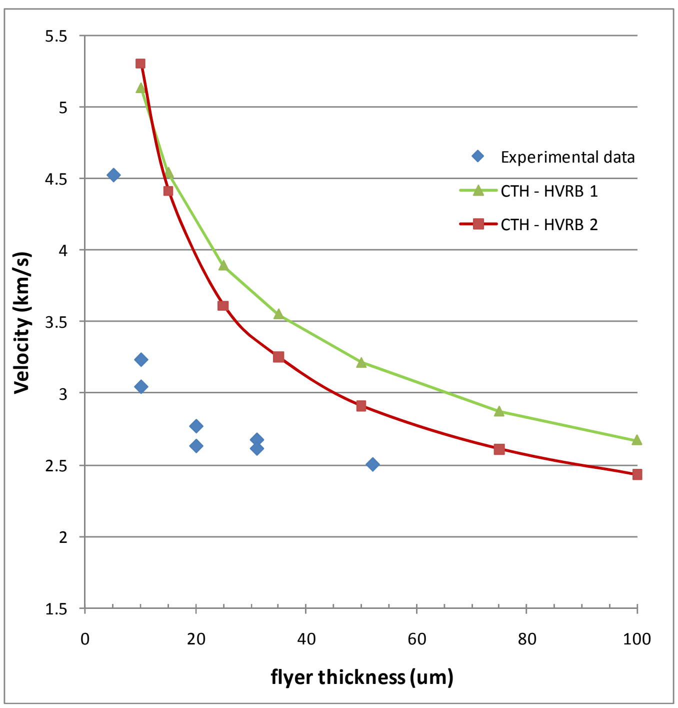
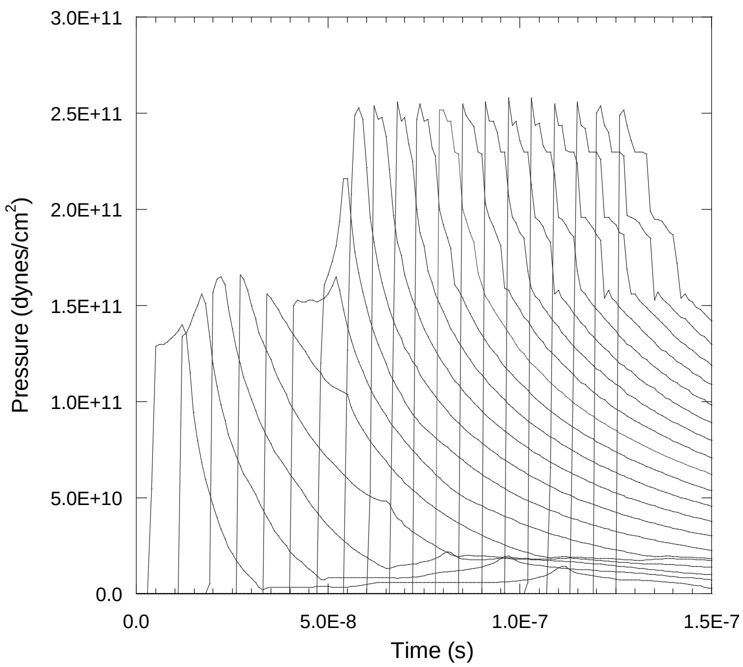


Figure 6. Threshold velocity for initiation by thin flyers. Both HVRB models over-predict the velocity.

Near the threshold for initiation, the run-distance can increase substantially beyond the sustained shock run distance. The two sets of parameters for the HVRB models above give two vastly different behaviors at near-threshold conditions. Figure 7 shows "HVRB 1" predictions of pressure-time profiles for impact by a 35µm thick flyer. The release wave from the back surface of the flyer catches the shock front approximately 30ns after impact. The pressure drops momentarily, but the reactions build up so fast due to the high pressures imparted by the flyer impact that the shock quickly transitions to detonation (at ~60 ns). In the model, the parameter, M = 1.5, causes the reaction to artificially lag behind the shock front, and the parameter, X = 1, allows the shock wave to almost instantaneously jump to detonation as the extent of reaction grows large.

The second model, "HVRB 2", does not impose a lag time on the reactions (M = 1.0); however, as the extent of reaction grows large, it is slightly inhibited by the larger value of X = 2.0. The net result is that the HE is slightly more sensitive to initiation (lower threshold velocity), but the transition to detonation occurs more slowly (~150 ns as seen in Figure 7). These are only two of many possible "paths" that the SDT process may follow. Knowing the details of the correct path becomes critically important when the model is extended from one dimension to two or three.



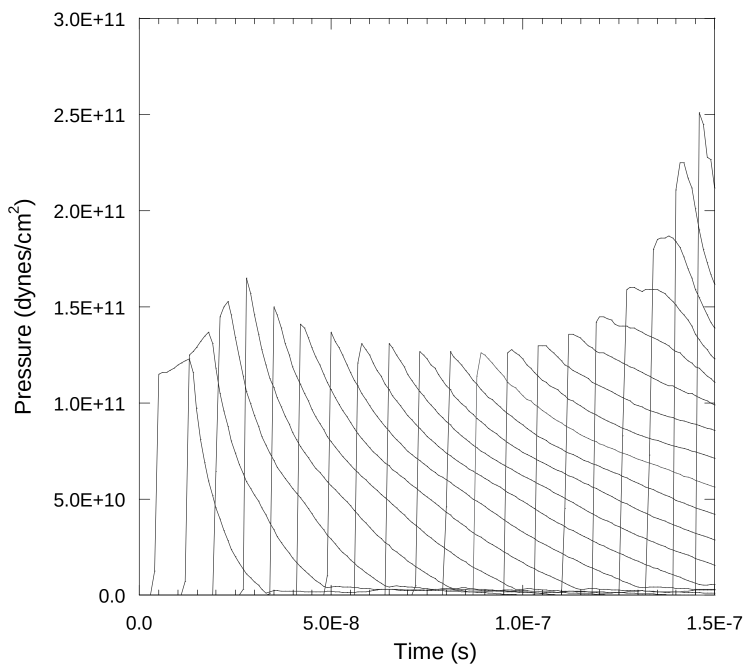


Figure 7. Pressure profiles predicted by the "HVRB 1" (top) and "HVRB 2" (bottom) models for a 35um thick flyer. The release wave catches up to the shock front within the first 30 ns for both cases. The shock wave is then sustained by reactions and grows to detonation in ~60 and 150 ns, respectively. In both cases, the flyer velocity is within 0.3% of the estimated threshold

2-D Model

If the run distance for initiation (ignition + transition) by a small spot sized flyer is sufficiently long, then the requirement of early time divergence during the ignition process driven by the impact shock wave causes the threshold velocity to increase. Also, as the spot size decreases, the diameter of the reacted region becomes smaller—to the point that it cannot sustain itself. The "minimum diameter" from which the HE can be shock-initiated may or may not be the same as the critical diameter for sustaining a pre-existing steady detonation as it does not capture divergence driven conditions and the underlying physical phenomena may be different in meaningful ways.

Figure 8 shows a 2-d axisymmetric simulation of impact on HNS by a 50 µm thick by 600 µm diameter flyer using the "HVRB 2" parameters given above. Although the impact pressure is sufficient to cause complete reaction of the material ($\lambda = 1$), the diameter of the reacted region is too small for the reaction to propagate. In reality flyers of much smaller diameter are able to initiate the material, and here again, the material is less sensitive than what is observed experimentally. The minimum diameter is very sensitive to the details of the transition to detonation and not just the sensitivity of the material. The "HVRB 1" model predicts that this material detonates with a flyer diameter of ~1mm at a threshold velocity only 5%greater than the 1-d prediction.

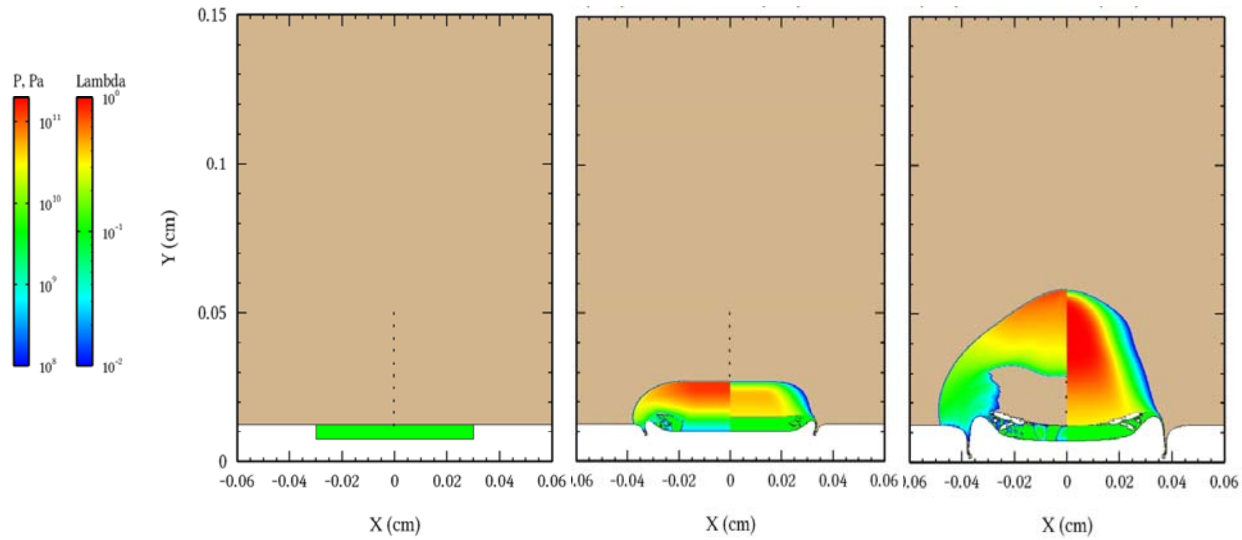


Figure 8. 2-d axisymmetric simulation of flyer impact into HNS. The left hand side of each plot (x<0) shows pressure, and the right hand side (x>0) shows the extent of reaction. Even though the flyer velocity is above the threshold for initiation (predicted by the 1-d model) and the material is completely reacted in a region approximately 200 µm diameter, the reaction fails to self-sustain and grow to detonation.

Conclusions

The ability of the HVRB model to make realistic predictions of thin-pulse initiation is being evaluated. Measurements of the pressure profiles during the run-up to detonation are needed in order to properly calibrate the model. In addition to the HVRB model, other reactive burn models, such as the Ignition Growth and Reactive Burn (IGRB) are being evaluated. A conclusion of the evaluation may be that the currently specified HVRB (and quite possibly other conventional reactive flow models) does not capture the phenomena imbedded within the experimental results and the fitted James paramaters. Consequently, additional focus must be applied to the validation of the James criterion, review of the ability of reactive flow models to predict that criterion and then the modification of those models as needed. Ultimately, mesoscale modeling efforts[14] may lead to the development of physically-based engineering SDT models by providing insight into the growth and coalescence of hotspots and the subsequent build up of energy in the shock front which leads to detonation.

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