LLNL-TR-737784

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Future Research Needed to Study the Response of an Explosive Assembly to Mechanical Insults

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August 30, 2017

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

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28 August 2017

1. Introduction

HE ignition caused by shear localization is the principal concern for safety analyses of postulated mechanical insults to explosive assemblies. Although prompt detonation from shock is certainly a concern, insults that lead to prompt detonation are associated with high velocity, and correspondingly rare. For high-density HMX assemblies, an impact speed (by a steel object) of 400 m/s is needed to develop a detonation in a run distance less than 30 mm. To achieve a steady plane shock, which results in the shortest run distance to detonation for a given peak pressure, the impactor diameter must exceed 60 mm, and thickness approach 20 mm. Thinner plates and/or smaller diameter ones require even higher impact velocity.

Ignitions from shear localization, however, have been observed from impacts less than 50 m/s in Steven tests, less than 30 m/s from spigot impact tests, and less than 10 m/s from various drop tests. This lower velocity range is much frequent in postulated mechanical insults. Preliminary computer simulations and analyses of a variety of such tests have suggested that although each is accompanied by shear localization, there are differing detailed mechanisms at work that cause the ignitions. We identify those mechanisms that may be at work in a variety of such tests, and suggest how models of shear ignition, such as HERMES, may be revised and calibrated to conform to experiment. We suggest combining additional experiments with computer simulations and model development to begin confirm or uncover mechanisms that may be at work in a specific postulated event.

2. Experimental ignition from low-speed impact

Ignition detection

In the past, for the Steven test, a *go* was recorded when the test fixture disassembled. The LLNL practice was to record a go when the blast gauges gave a signal. The AWE practice was to record a *go* when the test fixture disassembled or flames were observed coming from the vessel. In some cases, the AWE experience was that the blast gauges did not always report when the test fixture disassembled. A *no-go* left the fixture intact (although the cover plate was dented) with no measurable signal from the blast gauges. Localized ignitions that did not build up were not observable when the fixture remained intact, so not recorded as a *go*. Similarly, spigot impacts that left the target intact (except for the hole left by the spigot) may have shown discoloration when the target was examined post-test, but were considered ignitions, but without violence. A fast, high-resolution image (using for example a transparent back plate) might show light emission in both Steven and spigot tests at velocity below the *go* threshold. The refinement of the oblique impact test (skid test) at LANL also permitted the observation of transient ignition events that did not propagate. As a consequence the velocity for ignition, as now observed with new diagnostics, is lower than previously reported. Even drop hammer testing can be subject to reduced values of the drop height for ignition if the *go* is detected by light emission or detection of a few small product molecules, rather than by the amplitude of the recorded air-pressure (microphone output).

The challenge for a model used in computer simulations of the experiments is that the newly emerging requirement for the model is to not simply record when an ignition occurs, by whatever measure is used, but to also calculate the quantitative violence of the response. With this capability, confirmed by experiment, an appropriately conservative, rather than overly conservative, limit can be set on the specific mechanical insult to the specific explosive assembly under consideration. Assuming that the violence of an event can be calculated accurately enough, then the additional input required for the analysis of system is the violence that may be tolerated. The tolerable level will be negotiated by various interested parties, including stakeholders, and not necessarily an exclusively science- or engineering–based threshold.

The difficulty of the task of predicting quantitative violence levels should not be underestimated. The grail for thermal analyses of explosive systems is not just the time of reaction, but also the violence. For thermal analyses, the quest continues. Mechanical analyses have been under development for a much shorter time. Recently, a few crossover simulations, where calculations of violence from thermal events were successfully performed by carefully adapting models developed for mechanical analyses, have been reported.

Steven tests

We have noticed that the degree of shear localization in Steven test calculations is significantly affected by the choice of friction coefficient. There have been a few experiments at LLNL for obtaining the friction coefficient between several formulated explosives and various inert materials including Teflon and steel. For these materials, a single coefficient value of 0.4 seems to be adequate. As a result, all our reported Lagrange calculations of the Steven tests have used that value. As we noted, the experimental *go* from a Steven test requires the ignition to consume some of the explosive, break but do not shatter the confinement, and either produce air blast at some distance from the target assembly, or when cameras recorded flames, breaking up of the fixture, and/or a fireball. Ignition criteria based on comparison of Steven test results are, in fact, ignition with some accompanying growth of reaction. In the LLNL version of the test configuration, many LX and PBX formulations of CHE-based explosive show a relatively abrupt impact velocity transition between *no-go* and *go* of around 40 m/s. Steven tests with a transparent back plate have not been performed.

Spigot intrusion tests

Spigot intrusion tests simulations are most easily accomplished using an Eulerian formulation. In principle, an ALE formulation could be used, but calculations with a blunt nose are much more difficult to run to completion. Attempts at Lagrange simulations have proved fruitless. In many Eulerian formulations, including the formulation in ALE3D, there is no specialized treatment at material interfaces. Instead, mixed cells have a single velocity field. This is roughly equivalent to having a large friction coefficient, so that the explosive does not slip relative to the spigot. For that case, as with the case for finite but large friction coefficient, shear is localized near the interface.

In the UK, early spigot intrusion testing was done in an explosive assembly cup similar to the steel cup used for the UK variant of the Steven test. The spigot impacted bare explosive, but the surrounding assembly obscured the initial impact and partially confined the explosive. For those tests, a *go* was recorded using the same criteria as for the Steven test – breaking apart of the test vessel, flames, or fireball. In 2008/2009, spigot intrusion tests with a transparent back plate were carried out. For those tests, ignition was recorded by light output using a maximum framing rate of 24,000 fps. A few tests showed reaction through the window without the window breaking or test vehicle failure. Those tests would have otherwise been classified as *no-go*. The velocity needed to achieve reaction in these tests were higher than the velocity required for the tests with steel backing. The assumption is that the coefficient of friction for explosive on sapphire is smaller than explosive on steel. We note parenthetically that a new, faster camera with more pixels will record lower-levels of transient light than the old camera. The velocity threshold for ignition as determined by light emission will be on a downward trend as diagnostics improve.

Preliminary calculations of (older) spigot intrusion tests have resulted in similar ignition parameter values as those obtained at threshold velocity in Steven test simulations. The results have not been exact. A proper comparison would require simulations of the Steven test with the same mesh in Eulerian formulation. This has not yet been accomplished. Alternatively, an emerging ALE3D capability may be employed. This capability permits a Lagrange body (spigot) to move through an Eulerian target (explosive) with defined interface properties. Here, too the same capability would need to be used for both the Steven and spigot intrusion tests.

Spigot impacts with other confinement

Both LLNL and AWE have performed spigot impacts on small, test samples, lightly confined with Perspex. These calculations have shown ignitions, as diagnosed by light output, at lower impact velocity than the steel-confined tests. Light output when the spigot neared pinch at the back surface of the explosive occurred at 10 to 15 m/s impact velocity. Depending on the explosive, light output was also observed at the impact face, or for shallow penetrations before pinch. Tests with a short spigot, to preclude pinch, also showed ignitions at somewhat higher velocity than long spigot tests with the same explosive. We note that the velocity recorded for the spigot intrusion testing is usually the impact velocity. With light confinement, the spigot is not slowed appreciably in the process of explosive penetration. With heavier confinement and larger diameter spigots, the slowing was noticeable in the simulations and some early measurements.

Spigot intrusion with target perforation

A sequence of low speed, heavy drops (up to 6 m/s) was performed at AWE. In those tests, a spigot, placed at the surface of the explosive assembly was impacted by the dropping weight. The spigot perforated the test vehicle. In those tests where ignitions were observed, the origin seemed to be that the spigot caused petalling of the back plate, and rubbed the tips of the petals during exit from the target. Broken explosive extruded through the forming petals and/or was trapped between the spigot and the petals. Ignitions were observed there. It is uncertain whether this was due to heat transfer between the heated aluminium petals, or direct shear as the explosive was extruding. In no case did the ignition, observed on the high-speed cameras, propagate to the explosive assembly, and there was no observed ignition from the spray of broken explosive exiting the assembly as it impacted a steel plate located some distance from the back plate of the assembly. It is likely that this mechanism will be at work over a specific velocity range that depends on the back plate thickness and material properties. If the impact velocity is too slow, or the plate too thick, petals will not form. If the impact velocity is too fast, the petals will swing out of the spigot path and no longer remain in contact.

It is possible that a similar effect may occur during the perforation of the entrance plate of an explosive assembly, depending on nose shape. Flat spigots and thin front plates lead to front plate failure by shearing out a plug, rather than petalling. For that case, trapping explosive between spigot and the failure surfaces is unlikely. Ignitions that did not grow to violence would be obscured, and so not recorded. Additional testing and computer simulation on representative explosive assembly materials and geometry is needed to determine whether this mechanism is present for the assembly under consideration.

Ignition from oblique impacts

Analyses of the oblique impact test (skid test) results have demonstrated that the presence of grit with a suitably high melting point (and sufficient hardness) reduces the impact ignition velocity by a large factor. The recent, careful, experimental program at LANL used the expedient of gritting a glass plate, and photographing the event from behind to identify ignition by light output. The historic database used gritted steel plates and/or candidate flooring systems to be evaluated. Ignitions were recorded when an observable response – smoke or explosion, was filmed. Here again, the historic thresholds are based on a relatively sparse data set and produced more violence than when compared to the recording of light output. AWE has performed some small-scale trolley tests in which an explosive mass impacts an angled plate that is optionally gritted. When the plate was gritted glass, cameras viewing through the back of the plate recorded ignitions that failed to grow, so would have likely been missed were it not for the camera records.

Ignition from the drop hammer

Variants of the drop-hammer experiment are used in all explosive research laboratories as a small-scale screening test to determine the relative impact sensitivity of a new formulation. Ignitions are observed in drops from a few hundred mm to two meters, depending on the explosive formulation, each laboratory's apparatus, test protocol, and method of recording a *go*. At LLNL and other laboratories, the event is monitored with a microphone of specific sensitivity and mounted a specific distance from the sample to be tested. A sound level (blast wave) of a specific intensity is required to record a *go*. As a result, an ignition needs to be throughout (or propagate quickly throughout) a specific volume of explosive. In contrast, the apparatus used at Cambridge laboratory employed a glass anvil so that the ignition and ignition spread could be observed. Here, too, light output would be recorded as a go. However, the friction coefficient and surface roughness of a glass plate are sufficiently different from a steel anvil with a specified surface roughness or from a steel anvil faced with sandpaper of a certain grade and material (high melting point grit) that the drop heights for ignition will not be directly comparable.

3. Model requirements for low-speed ignition

Ignition associated with shear localization

Shear localization is a result of mechanical instability brought on by a decreasing resistance with increased load. This can occur as a result of decreasing area, such as the neck that develops in a simple tension test, or of damage build up, such as can occur with granular materials. Thermal softening, too, can lead to the severe localization of a shear band, where only thermal conductivity can increase the shear band thickness that otherwise would occur. As a consequence, for the computer simulation to produce accurate localization of the strain field, the constitutive model for strength must be accurate. Since formulated explosives are granular materials with visco-elastic/visco-plastic binders, the strength increases with confining pressure and strain rate and strain, and decreases with damage (and temperature build-up). This, in turn, requires a suite of experiments at the strain rates and confining pressures that are observed in simulations of the various ignition tests.

If the model for ignition is chosen to be thermal, and based on measurement of runaway in thermal experiments, then the requirement of the model is to not only to get the location and degree of shear localization correctly, but also calculate the time at temperature correctly. The HERMES model (see the appendix) seeks to simplify the calculation of ignition by a phenomenological model. It posits that ignition occurs where shear is localized, and the value of a measure of localization is treated as a threshold trigger.

In any event, limited information will available to set the parameters of the constitutive model, perhaps only by analogy with other, similar explosives. Various postulated insults and ignition tests are simulated and the results examined. Additional experiments at additional and appropriate confining pressures and strain rates may be needed. To the extent that the experiments and the postulated insults result in similar loading conditions, the calculated threshold values are likely to be close enough that specific, new experiments can be designed, tested, and the model results assessed. The constitutive model need not be precise, so long as the loading and loading rates in the test used for calibrating ignition and the loading rates in the postulated insult scenario are the same near the ignition region. To the extent that the loading and loading rates differ, additional experiments may be required. Comparison should also be made to the loading and loading rates used to define parameters in the constitutive model. Here, too, significant differences may require additional experiments to refine constitutive model parameters.

Ignition associated with grit

The large-scale oblique impact (skid) tests have clearly shown the importance of the presence of high melting point grit on the threshold impact velocity for ignition. This is also observed, although not as clear-cut as one could wish, in the very small scale drop hammer tests, where the condition of the anvil has an important influence on the drop height. Directly modelling the influence of grit would doubtless prove to be research project of its own. The grit dimensions are comparable to the explosive crystallite dimensions. In that case, it is unlikely that the macroscale friction coefficient would have any bearing on the mesoscale interaction of grit with explosive crystallites and binder, including binder adhesion.

As an alternative, consider continuum experiments to measure the friction coefficient of explosive and confinement materials in the presence of grit with an appropriate surface density. This revised friction coefficient can then be used in continuum simulations of the ignition experiments, and a revised (smaller) critical ignition parameter obtained. This revised value would then be used in postulated insults where grit is known to be present (or suspected to be present).

In addition, it is possible that smaller scale tests could be used to establish an ignition threshold in the presence of grit. The Steven test is a plausible candidate, with the addition of the same surface density of grit to see if those Steven test velocity threshold is affected. In that test, there is a limited amount of slip between the back surface of the explosive disk and the steel cup that holds it. That, in turn, may reduce the effect of grit on the threshold velocity. It is possible that eliminating the Teflon retaining ring would give additional distance for slip. Computer simulations may guide this aspect of the modified test design. In addition, the result of comparing experiment with simulations may guide the next generation of models for ignition with grit.

Ignition associated with confinement failure

The observation of the very low-speed ignition near the interaction zone of a perforating spigot and the failing back plate of the explosive confinement suggests that this may be an important mechanism. Although those ignitions were not accompanied by significant growth of reaction, it is possible that such a growth to violence could occur in other geometries. As a rule, calculations of target perforation are best done in Eulerian or ALE formulations. However, accurate fracture modelling remains a research study on its own. The requirement for studying ignition near the spigot back plate interaction does not necessarily require accurate modelling of the number of petals, only that there are some and they retain appropriate contact with the spigot as it passes through. Specific experiments looking at the behaviour of candidate back-face materials in this regime of low-speed perforation should be performed to see whether entire classes of materials could be eliminated because their failure modes are different. At that point a strategic decision can be made as to whether materials that fail and produce ignitions are candidate materials for explosive assemblies for which insults are postulated.

4. Model requirements for the transition from ignition to violence

Conductive burn

Conductive burn has been measure by several different laboratories for a variety of formulated explosives. The results for undamaged material are all relatively similar in that the burn speed is observed to be roughly linear in pressure from one bar to a few kbars. This dramatic increase in burn speed is the result of the hot, compressible gas products staying much closer to the burn front at high pressure with the resulting increase in heat transfer.

Convective burn

Although probably misnamed, the observation of a much faster transfer of hot gas through damaged material with connected porosity is clear. The advance of the flame front through the porous bed depends hydraulic radius of the paths between broken particles and the transport properties of the hot gas products. In principle, it also will depend on the pressure gradient that drives the hot gas, and the ignition dynamics of the surfaces those hot gasses find. There are limited data upon which to build a model, and no data on the evolution of pressure in a burning, damaged volume.

Specific, focused experiments are needed in a simplified geometry where the flame can advance from a well-defined ignition site and the dynamic pressure rise recorded. These experiments are essentially unrelated to ignition experiments. In that regard, they are more akin to DDT experiments, except that the objective is not to run to detonation but rather to observe the build up of pressure following a well-understood and well-diagnosed ignition. Since these experiments could be performed with explosive material of known surface area (from separate burn rate measurements) and porosity, those parameters could be independently changed to establish the experimental dependence of the pressure build-up.

Finally, the complete set of experiments would include experiments to quantify the damage (specific surface area and porosity) caused by a mechanical insult. This is a much larger suite of experiments and computer simulations and model development than would be the case if the threshold of ignition were not so different from the threshold for unacceptable violence.

Alternative to calculating violence

An alternative to this extra burden of experiment and model capability is to revert to ignition criteria that only consider an ignition to have happened if it is accompanied by enough growth of reaction to produce an unacceptably violent event. In this way, models that are calibrated to ignition events with this new (old) definition can be used to demark acceptable response from unacceptable response directly without having the challenge of accurate calculation of the growth of violence.

5. Summary

Ignition

The constitutive model of the explosive, and to a lesser extent the constitutive models of the confinement materials, are dominant in determining the localization of shear resulting from a specific mechanical insult. If the shear localization is sufficient, as determined by experiment, ignition occurs. In practice, the constitutive model is fitted to results from a limited number of different experiments on the same or at least mechanically similar explosive. Provided that the range of loading and loading rates in the mechanical property tests are representative of the loading and loading rates that occur in the postulated insults, the calculated localization will be accurate. If the property tests are not over sufficient range of loads and rates, then additional testing may be required.

For some tests designed to measure ignition thresholds, the reported threshold is for ignition that develops into some measure of violence. For other, more recent test and diagnostics, ignitions are observed that do not propagate, and are benign. Here the analyst and experimentalist must work closely to make sure that both are aware of the limitations of the experimental techniques and diagnostics.

Acceptable response for ignitions that grow

All interested parties must agree on whether ignitions that do not propagate are unacceptable, or whether ignitions must propagate and result in some external measure of explosive response may be accepted. All parties must acknowledge that there is risk associated with any decision. If the decision is to err on the side of too conservative, so that benign ignitions are ruled unacceptable, there will be additional costs required to prevent low-level insults. These costs may be significant. On the other hand, if in some cases ignitions grow too aggressively, there is the cost associated with post-event damage control. We note that historically, the ignition thresholds that have been reported included some growth of reaction.

Ignitions that grow

If the decision that some growth of reaction is acceptable, then specific experiments with accompanying simulations and model development must be targeted to develop a quantitative understanding of the factors that permit growth of the reaction, the acceleration of that growth, and the factors that slow down and stop the reaction from growing. Since this aspect of explosive assembly response has not been previously required, careful planning, diagnostics, and execution of the experiments will proceed hand in hand with computer simulation. This presents an opportunity for difficult, important, and ultimately rewarding research.

Acknowledgement

Andy Jones, AWE, provided helpful comments about the experiments performed at AWE and their interpretation of the results.

Appendix: HERMES ignition parameter

The HERMES ignition parameter was developed in preliminary form in 2008 and in its present form in 2009. The parameter identifies local domains where shear strain (as distinguished from plastic strain) is large and coupled with compressive stress normal to the shear plane. The HERMES ignition parameter is given by

$$I_{gn} = \int_0^t \left(2 - \frac{27|s_1 s_2 s_3|}{2Y^3}\right)^5 \left(\frac{p + s_2/2}{P_0}\right)^{1/2} \dot{\varepsilon}_p dt \tag{1}$$

where s_i are the ordered principal stress deviators, p is the mean stress, Y is the yield stress (proportional to the second invariant of the stress deviator tensor) ε_p is the equivalent plastic strain, and P_0 is a parameter. Since the plastic strain rates are proportional to the stress tensor, according to the plastic potential flow rule, the first bracket weights the integral when plastic strain is developed in pure shear ($s_2 = 0$) compared to plastic strain developed in compression or tension where two of the stress deviator tensors are equal, making the second term in the first bracket unity. The power, chosen to be 5, makes the weighting ratio 32 to 1. The second bracket weights the integral when the stress normal to the plane of maximum shear is compressive. For the most part there is only one test geometry for which the ignition parameter has been calibrated. As a result, the two powers and P_0 (taken as 5 kbar) have never been changed. Instead the single parameter for a mesh-resolved Steven test, is chosen by calculating the maximum value in the mesh that obtains at the measured velocity threshold for *go/no-go*.

Shear strain can localize as a result of softening, which can be caused by temperature or damage. In the model, however, thermal softening is not permitted to occur. If it were included, shear would localize in a shear band, which has a thickness limited by heat transfer. In metals the shear bands are "large," of order microns. Comparable shear bands in a poorly conducting explosive are orders of magnitude smaller. (For the moment, we are here ignoring the heterogeneity of explosive assemblies and considering the material to be represented by continuum variables.) We further note that an ignition criterion that uses thermally driven kinetic rates would require resolving the shear bands.

In HERMES shear localization is analogous to the boundary layer in fluid mechanics. In the explosive, the rate-and pressure-dependent strength plays the role of viscosity. We have observed a characteristic boundary layer thickness of 100 microns in our calculations. Plastic strain decreases exponentially with distance from the boundary. If the mesh resolution is much coarser than the characteristic dimension, the calculation will not capture the maximum value of the ignition parameter. The expedient solution is to reduce the criterion value for the ignition parameter to one appropriate for the mesh resolution that can be afforded for the specific calculation.