Title: HIGH EXPLOSIVE VIOLENT REACTION (HEVR) FROM SLOW HEATING CONDITIONS

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HIGH EXPLOSIVE VIOLENT REACTION (HEVR) FROM SLOW HEATING CONDITIONS

ABSTRACT

The high explosives (HEs) developed and used at the Los Alamos National Laboratory are designed to be insensitive to impact and thermal insults under all but the most extreme conditions. Nevertheless, violent reactions do occasionally occur when HE is involved in an accident. The HE response is closely dependent on the type of external stimulus that initiates the reaction. For example, fast heating of conventional HE will probably result in fairly benign burning, while long-term, slow heating of conventional HE is more likely to produce an HEVR that will do much more damage to the immediate surroundings. An HEVR (High Explosive Violent Reaction) can be defined as the rapid release of energy from an explosive that ranges from slightly faster than a deflagration (very rapid burning) to a reaction that approaches a detonation. A number of thermal analyses have been done to determine slow heat/cook-off conditions that produce HE self-heating that can build up to a catastrophic runaway reaction. I will specify the conditions that control reaction violence, describe experiments that produced an HEVR, describe analyses done to determine a heating rate threshold for HEVR, and list possible HEVR situations.

DEFINITION OF HEVR

A high explosive violent reaction (HEVR) can be defined as an explosion or a rapid release of energy whose reaction rate ranges from slightly faster than a deflagration (extreme rapid HE burning) to one that approaches a detonation. HEVR in conventional high explosives (CHE's) such as HMX (high melting explosive), can have a power output that varies over many orders of magnitude. This is illustrated by the power-energy comparison of a detonation, an explosive burn, and a fuel oil-air burn [1]. Although the energy output of fuel oil is approximately ten times greater than that of HE, a fuel oil-air burn reacts at a rate less than 1 mm/s, compared to an HE detonation whose reaction rate can be as high as 7000 m/s. The power output of an HEVR in CHE can range from $10^3$ to $10^9$ watts/cm$^3$. The power output of insensitive high explosives (IHE's), specifically, TATB (1,3,5-trinitrobenzene) formulations, has never been observed to transit to violent reaction as a result of thermal ignition.

While HEVR has been demonstrated in thermal stimulus tests of CHEs, a detonation has never been verified. The reaction, although very violent, may not be a true detonation; that is, the same pressure/time energy deposition as an intentional detonation.
is not delivered to the surrounding components. Hence, the term HEVR is used in this report.

WHAT CONTROLS REACTION VIOLENCE?

HEVR depends on the following: 1) HE formulation, 2) degree of confinement (high confinement favors HEVR), 3) size and geometry (larger size favors HEVR), and 4) location of initial ignition (interior ignition, which can be controlled by changing the heating rate, favors HEVR). HMX-based explosives have been shown to HEVR, but different formulations (binders, plasticizers) display different sensitivity and propensity to HEVR. Fast heating of bare HE charges will cause ignition on the outer surface of the HE, probably resulting in burning, or at most, deflagration. In fact, large bare HE charges are routinely disposed of by open air burning, resulting in nonviolent reactions. Slow heating of conventional high explosives is more likely to ignite internal to the HE charge, more likely to result in bulk heating of the HE, allow a pressure buildup through self-confinement, and make HEVR possible. A runaway reaction will always begin at the hottest point in the HE, defined by the heat path and rate, determined by the geometry and temperature history of the device.

A series of tests were performed at Los Alamos on small bare HE spheres of the CHE, PBX 9501 (95/2.5/2.5 wt.% HMX/Estane/BNDPA-F), and the IHE, PBX 9502 (95/5 wt.% TATB/KELF-800), that reveal important basic thermal properties [2]. Both PBX 9501 and PBX 9502, like all explosives, have a critical temperature, above which, the HE decomposition rate accelerates after an induction (time delay) period. The critical temperature is defined as the lowest constant surface temperature at which a specific material of a specific size and shape will self-heat catastrophically. When the boundary temperature is raised rapidly above the critical temperature, only the surface material goes through a short induction phase and reacts by a deflagration mechanism. However, in a slow heat environment, the temperature inside the HE volume will be higher than the boundary temperature because of its internal decomposition reaction. Although no violent reactions were observed in these small tests, if a significant volume of the charge is held close to the critical temperature, a run-away reaction can build from an ignition point rapidly enough to cause HEVR in large, unconfined CHE charges.

The critical temperature curves for various explosives commonly used at Los Alamos [3 and 4] show that IHE (TATB formulation) has a much higher critical temperature than the conventional HEs and that critical temperature rapidly decreases as explosive size increases. Theoretically, a large enough piece of HE could self-ignite at room temperature.

EXPERIMENTS THAT PRODUCED HEVR

The most complete and thorough cook-off tests performed to date, as far as diagnostics are concerned, were done at Livermore by S. Chidester, et al., [5]. A series of twenty cylindrical tests were done on HMX and TATB based explosives to measure the degree of violence that can be obtained from HE exposed to a purely thermal stimulus.
The HE in these experiments consisted of either hollow or solid cylinders confined by steel and aluminum shells that were slowly heated by a number of heating bands. The violence of the reaction was measured using thermocouples, timing pins, pressure gauges, shrapnel tanks, witness plates, and dual pulse flash x-ray photography. These experiments were important in that they showed no evidence of reactions which transition from thermal ignition to detonation.

The LANL Slow Heat Test, which subjected lightly-confined, live CHE charges to a worst case heating condition that was far more severe than any Stockpile-to-Target Sequence scenario, was intended as a severe over-test with a high payoff. Realistic confinement was achieved by putting CHE charges inside a sealed containment vessel. The containment vessel was placed inside a disposable oven and slowly heated by means of four electric heaters. A catastrophic thermal runaway reaction occurred after several hours of heating, producing an extremely violent reaction, just the opposite of what we hoped for. We were able to calculate the correct time and temperature to the runaway reaction in the HE and determine the location of initial buildup to catastrophic self-heating in our post-test analysis. This test showed that we were overly optimistic of the results of a high-risk experiment.

Another test used by LANL to characterize susceptibility of explosives to HEVR is the Heavily Confined Heating Test [6]. In this test, a 3-kg spherical charge of HE is placed in a sealed, steel vessel assembly with 51-mm-thick walls and an end cap held on with bolts designed to fail in tension at 40,000 psi internal pressure. Heating tape is placed around the vessel and the assembly is heated at a rate of 45°C/hr., until a reaction occurs. The violence of the reaction is judged by the fragment sizes of the vessel recovered after the test. Heavily Confined Heating tests were conducted on various HE formulations, including HMX-based and TATB-based explosives. The results showed a clear difference between the explosives; similar HMX-based HEs with slightly different formulations (binders, plasticizers) exhibited vastly different behavior and propensity to HEVR. PBX 9501 always reacted less violently than the other HMX-based HEs in these tests.

**DETERMINING A HEATING RATE THRESHOLD FOR HEVR**

I used the ABAQUS computer code [7] to calculate the thermal response of the PBX 9501 tests described above. ABAQUS is a general purpose, finite element code that is commercially available from Hibbitt, Karlsson, and Sorensen, Inc. It has been modified with a user subroutine that allows us to predict the time and temperature of a runaway reaction in HE. I made an axisymmetric finite element model of the Heavily Confined Heating Test device and subjected it to the observed heating conditions. My analysis, using temperature data measured at the outside surface of the vessel as input, indicates that thermal ignition occurred at a point 1 mm from the outside surface of the HE sphere. This ignition depth might be used as a threshold that bounds the less violent end of the HEVR spectrum for PBX 9501.

I also did a series of analyses to determine the depth of ignition and time to a runaway reaction in cased PBX 9501 exposed to various slow heating conditions. My goals were to determine the effect different heating rates have on the depth of ignition of
PBX 9501 and to calculate the minimum time required to obtain in-depth ignition in cased HE. I did a parametric study on a spherical model of a lightly cased HE assembly using: 1) Arrhenius kinetics with and without an induction (time delay) term, 2) heating environments severe enough to cause HE ignition in times as short as a few minutes to as long as several hours, and 3) fine-to-coarse modeling of the HE layer.

I used the EXPLO computer code [8] for this analysis. EXPLO is a one-dimensional, thermal analysis code that allows us to use temperature dependant properties and multiple heat source terms with temperature, flux, convection, or radiation boundary conditions. EXPLO uses N-th order Arrhenius kinetics and the finite difference method to calculate temperature fields and time to initiation for explosive materials. Our PBX 9501 model uses kinetic constants derived from modified Henkin test data [9] and 1-inch diameter spherical HE charge experiments [2].

Using a one-dimensional spherical model of a confined HE system, I did a series of analyses applying a constant flux boundary condition on the inside of the HE, and a progressively higher fixed temperature boundary condition on the outer case. In another series, I raised the ambient air temperature outside the case and allowed convection and radiation from the case surface using a spectral emissivity of 0.9. I used EXPLO to calculate the time to HE ignition and the distance of the ignition point from the HE surface (ignition depth) for the different constant boundary temperatures. The thermal analysis results and the available test data indicate that a fairly slow heating rate is required to produce HEVR in PBX 9501. The evidence indicates that under these conditions, the thermal environment is a “slow heating” event (may produce HEVR) if ignition occurs at a depth greater than 1 mm. I also postulate that a thermal environment is a “slow heating” event if heating duration exceeds one hour.

Past experience indicates slow heat/cook-off environments or accidents severe enough to cause an HEVR are uncommon, but several possible slow heat scenarios include: shipping containers or protective insulation layers that restrict the outward flow of heat produced by materials that undergo radioactive decay, fire fighting procedures that allow long-term fires to feed heat into HE for many hours, and environmental tests where a temperature-control system malfunction is possible.

CONCLUSIONS

We need a fundamental understanding of how slow heat explosions develop using basic experiments, improved computer models, and full-scale tests. We can accurately predict the time and temperature of a runaway reaction in HE, but not the violence. Tactical test parameters must duplicate an HE system’s explosive size, geometry and confinement, in order to accurately determine the fastest heating rate that will produce an HEVR; and even then, in some cases a somewhat subjective assessment will have to be made on whether the HE response is an HEVR, or simply deflagration. Because a substantial HEVR can be obtained from purely thermal stimulus in a lightly confined HE system containing PBX 9501, more testing, with proper diagnostics, is required to characterize the nature of HEVR and to compare the reaction violence of both weak and extremely energetic HEVRs with that obtained in a detonation.
REFERENCES


7. ABAQUS/Standard computer code provided by Hibbitt, Karlsson & Sorensen, Inc., 1080 Main Street, Pawtucket, RI, 02086-4847.
