

Shear Reaction of Explosives and Propellants

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ABSTRACT

When loaded by weak impact, both explosives and propellants undergo shear reaction. Our shear reaction hydro-reactive model (TDSR) is similar to our old surface burn hydro-reactive model (TDRR), except for the reaction rate equation. We perform tests and computer simulations of shear reaction in both explosives and propellants. For explosives we use the well-known Steven test but with different diagnostics (back surface velocity histories). For propellants we use a new test configuration. In both cases we run our TDSR simulations and are able to get a reasonable reproduction of test results.

INTRODUCTION

We're considering here initiation and reaction of explosives and propellants from weak impact loading, where the main response is in shear.

There are several kinds of initiation and reaction, according to the structure and mechanical properties of the energetic material. For each of those kinds, the macroscopic response (which is what we observe in tests and in computer simulations) depends on what is happening inside a representative control volume, or inside a computational cell, i.e., on the mesoscale. The two main kinds of initiation and reaction are surface burn [1-3] and bulk reaction [4]. Surface burn results from thermal localization, when reaction is ignited at discrete points in the considered cell. Those ignition points are known as hot spots or ignition sights. Reaction may then spread out of those ignition sights by means of burn waves, and when pressure is involved, by means of deflagration waves. Bulk reaction may occur when there is no thermal localization, and reaction is ignited throughout the cell volume, upon passage of the loading wave. When surface burn occurs, burn or deflagration fronts separate the reaction products from the reactant, and each of them is at a different temperature. When bulk reaction occurs, the reactant and products are all the time in intimate contact, and their temperatures are equal or almost equal. Those differences between surface burn and bulk reaction make their mix rules (that translate from the mesoscale to the macroscale) quite different. Surface burn may happen when: 1) the energetic material is somewhat porous; 2) the energetic material is a viscoplastic solid, or 3) both. When the energetic material is porous, pores may collapse under pressure to create ignition sites. The pressure needed for such an ignition is above about 2 GPa for secondary explosives, and the ignition duration is quite short, several ns. With our surface burn reactive flow model (TDRR=Temperature Dependent Reaction Rate) [1-2], we usually ignore the pore collapse duration. When the energetic material is a viscoplastic solid (a solid with strength that flows under shear loading), it may undergo shear localization (formation of shear surfaces or shear bands) [5-7]. Shear localization may lead to substantial heating over a narrow volume, leading to ignition. The ignition threshold of this mechanism is rather low (see later), and the related time to ignition is rather long, about 50 μ s (see later). From the properties of these two

ignition-mechanisms we may conclude that: 1) for a low velocity impact, shear reaction may ignite first. If as a result the cell pressure rises to cross the pore collapse threshold, pore collapse reaction may ignite and take over, being much faster; 2) for a high velocity impact, the pore collapse reaction, being faster, happens first, and shear reaction does not come about. But if the energetic material is a viscoplastic non-porous solid, shear reaction may ignite (through formation of shear bands) and then develop into full detonation. We refer to the shear reaction model as TDSR (=Temperature Dependent Shear Reaction). As TDRR and TDSR both deal with expansion of deflagration waves from ignition sights on the mesoscale, their rate equations are identical, and they differ only in terms of their ignition thresholds and rate equations.

Bulk reaction happens when there are no possibilities for thermal localization, which means that the energetic material is homogeneous (without pores) and with no strength. The classical case of bulk reaction is a liquid explosive without bubbles [4]. The ignition threshold of bulk reaction is rather high, because its ignition temperature depends on shock heating. In liquid explosives like nitromethane, the ignition shock pressure threshold is about 8 GPa. Correspondingly, its ignition duration is rather short, of the order of shock transition.

We're dealing here with weak impact, the response of which has mainly to do with safety aspects. As safety aspects get generally less attention than performance aspects, the current state of knowledge on the response to weak impact is lacking. The level of precision needed on the response to weak impact is rather low, because of the uncertainty concerning events that cause safety problems. As a result, the margin of safety usually taken for safety problems is large, and we allow for them a sizable error. This is in contrast to performance problems where we seek good precision.

Response of explosives to low velocity impact

There are several formats of low velocity impact tests that have been developed in various labs during the years, and we're not reviewing those here. One of them, developed in Livermore labs some 25 years ago and has been quite popular, is known as the Steven test, named after its developer [8]. In Fig. 1 we show a schematic plot of this test.

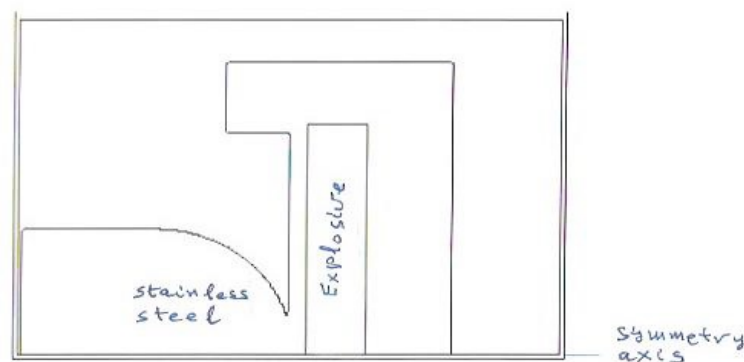


Figure 1. Schematics of the Steven test configuration.

The Steven test configuration includes a stainless-steel projectile 60 mm long and 60 mm in diameter, with a semi-spherical head. The projectile is accelerated by a laboratory gun

projectile to a velocity of several tens of m/s to about 200m/s, into the center of the sample target. The energetic material being tested has the shape of a disc, 120 mm in diameter and 14 mm thick. It's held between two stainless steel discs, a 4 mm forward disc and a 19 mm backward disc. The discs are closed radially by a stainless-steel ring, and there's a small gap between the energetic material and the ring. The original diagnostics of the Steven test are blast gauges at a distance of about 3m from the explosive sample. Trying to use those diagnostics, we concluded long ago that they are not good enough, and we're using instead particle velocity gauges on the back boundary of the target. We simulate the Steven test computationally using our TDSR model. As mentioned above, TDSR differs from TDRR in two respects: 1) ignition threshold; and 2) reaction rate equation. The ignition criterion of TDSR (shear ignition) is:

$$PD=(PD)_{\text{ign}} \quad (1)$$

Where P is pressure and D is effective strain rate. This criterion is based on experimental work from the 1950s [9], from which it becomes clear that ignition threshold of explosives from shear loading goes up with strength. As is well known, the main characteristics of explosives in terms of their strength are: 1) strength increases with pressure; 2) strength increases with strain rate, and 3) strength decreases with temperature. But temperature change from a weak impact is minor, and may be ignored when considering ignition threshold. Finally, as shear ignition threshold (or shear bands formation threshold) increases with strength, it increases with pressure and strain rate, and to a first approximation it increases with their product.

In the past we calibrated ignition threshold of an HMX based explosive from published Steven test results [3]. The calibration procedure is: 1) perform Steven tests with various impact velocities to determine the ignition threshold impact velocity u_{ign} ; 2) run a simulation of the test for u_{ign} ; 3) at the end of each time step write down the maximal value of PD over the explosive cells ($PD_{\text{max}}(t)$); 4) the maximal value thus obtained is the ignition threshold, $(PD)_{\text{ign}}=\max[PD_{\text{max}}(t)]$; 5) Later we improved the ignition threshold definition as follows: ignition threshold is the maximal value of PD that holds at least some assigned time which we call stay time. The ignition criterion that we calibrated in this way is $(PD)_{\text{ign}}=0.0075 \text{ GPa}/\mu\text{s}$.

As explained above, shear ignition may result from shear localization by the formation of shear bands. We're able to simulate the formation of shear bands with the appropriate resolution in a 1D computation of torsion of a thin-walled tube [7]. Tests of this configuration were performed on steel tubes [10], and in these tests they were able to observe the shear bands and measure the shear band temperature. We used our simulation code to reproduce those test results, thereby validating our computations. We then used those computations to predict the formation of shear bands in thin-walled tubes made of an HMX explosive, and in the next figures we show results of such computations. We show temperature profiles at different times and the temperature history at the shear band. The ignition temperature of the explosive in Figs, 2 and 3 (HMX+10% Viton) is about 550K, and according to Fig. 3 this temperature is reached after about 70 μs , which is the right order of magnitude. We show later that the ignition time (t_D) that we calibrated from Steven tests is only 50 μs , but this is good enough, as the explosive strength model that we use is not fully calibrated.

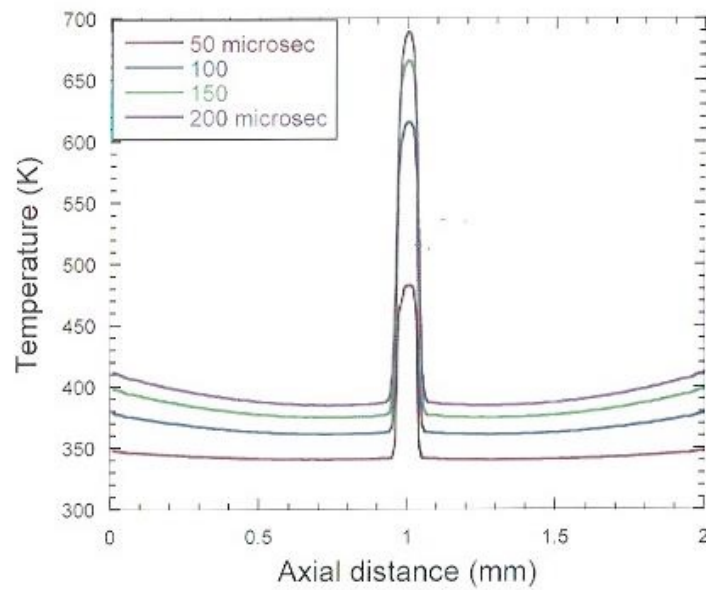


Figure 2. Temperature profiles along the tube at 4 times

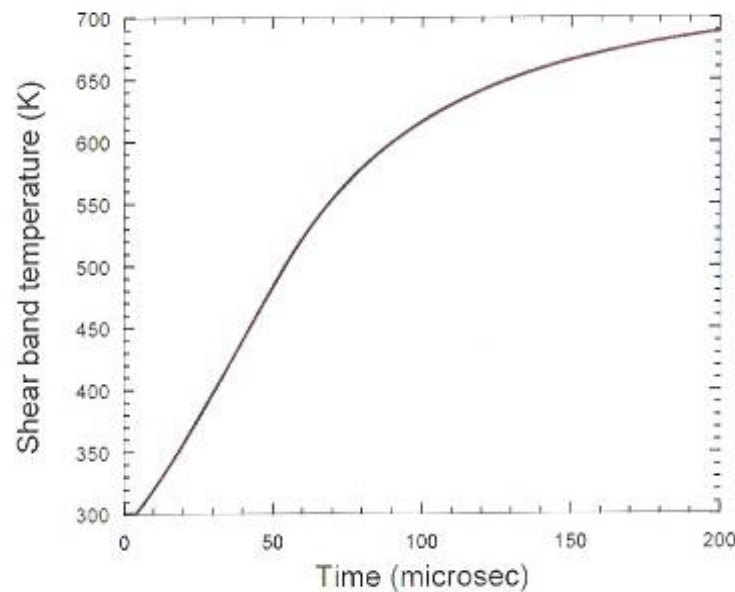


Figure 3. Temperature history at the center of the shear band

The reaction rate equation that we use with TDSR differs from the equation we use with TDRR only by its pressure dependence. The reaction rate equation is:

$$\dot{W} = R_{SB} P y(W) \exp\left(-\frac{T^*}{T_s}\right) \quad (2)$$

Where the index SB stands for 'shear bands' and replaces the index T in the reaction rate equation of our TDRR model, where T_s is the temperature of the unreacted (solid) part, and W

is the relative amount of reacted material. The burn topology function $y(W)$ and the parameter T^* we leave as in TDRR, as long as we don't have test data that require to change them. The reasons for including pressure dependence are: 1) from burn velocity measurements at temperatures close to room temperature it is known that burn velocity is approximately linear with pressure. This is because at this temperature the explosive is gaseous, and because reaction duration is long. Also, the explosive thickness perpendicular to the burn direction is changing with an inverse relation to pressure, and the rate of heat transfer is therefore increasing linearly with pressure. For the Steven test pressure is low, just a fraction of a GPa; 2) when pressure is high (like from a shock), volume change with pressure becomes less important because of shock heating, and the temperature part of the reaction rate equation becomes more important; 3) In recent years measurements of deflagration velocity of various explosives at room temperature and under high pressure have been made in a diamond anvil cell [11]. We show results of those measurements in Fig. 4.

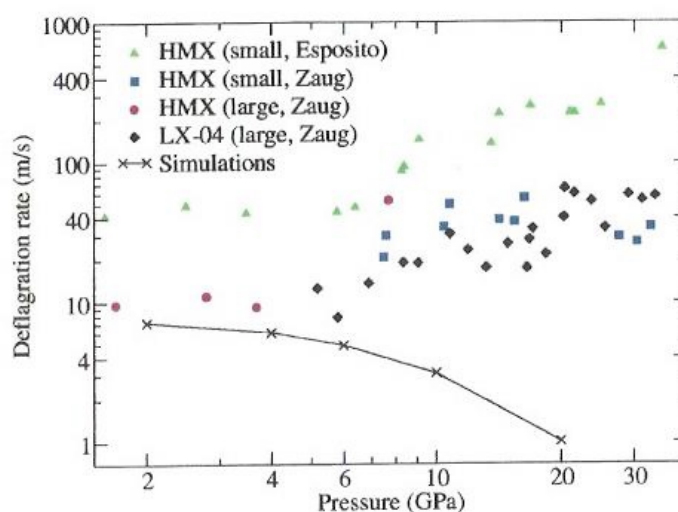


Figure 4. Deflagration velocity of several explosives as function of pressure from measurements in a diamond anvil cell. Line in the figure is from simulations by a group in England.

We see from Fig. 4 that our assumption about the influence of pressure on reaction rate does come about in the tests, but to a lesser extent. Above a pressure of about 1 GPa, deflagration rate is indeed increasing with pressure, but at a rate that is somewhat lower than linear. We also see that whoever did the simulations in England (line in the figure) was quite off truck.

We performed Steven tests as described above. The explosive was PBX 9501 (=HV10=90%HMX+10%Viton), and the velocity gauges were placed at 3 radii: 10, 25 and 40mm. We show the results in Fig. 5.

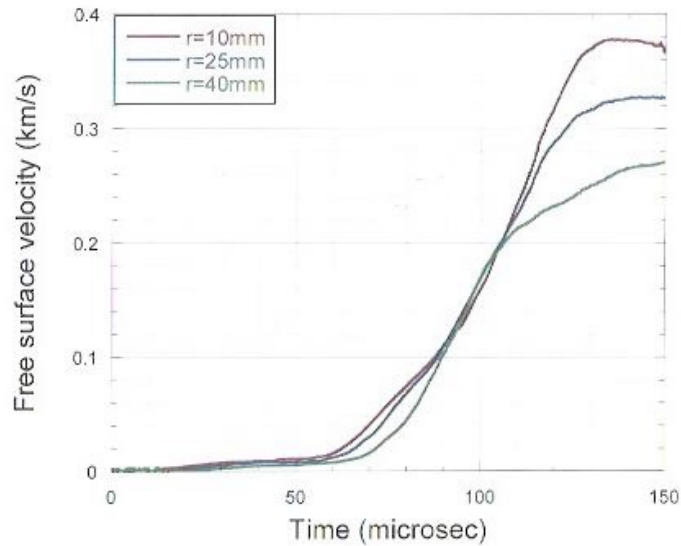


Figure 5. Measured histories of back boundary velocities at 3 radii, from Steven tests with the explosive PBX9501. The impact velocity is 120 m/s

In Fig. 6 we show our simulation results, and in Fig. 7 we compare test results to simulations for each gauge separately. The parameters we use in the simulations are: $R_{SB}=25.2/\text{GPa}/\mu\text{s}$, t_D (delay time) $=50\mu\text{s}$.

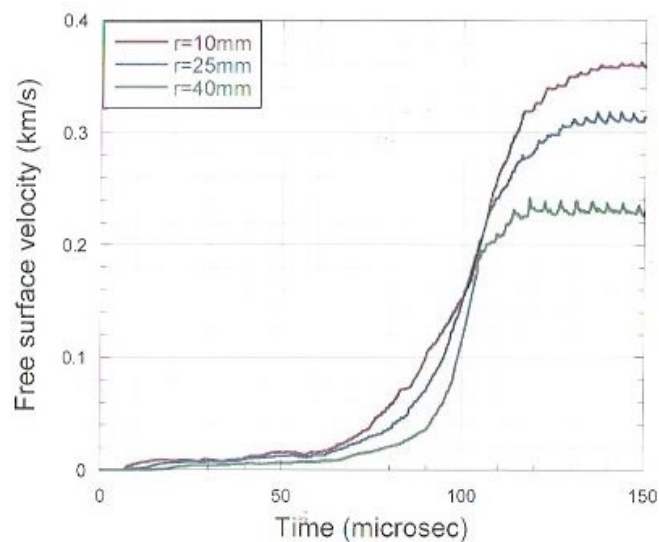


Figure 6. Computed results of the back surface velocity at three radial distances of a Steven test. The explosive is PBX9501 and the impact velocity is 120 m/s.

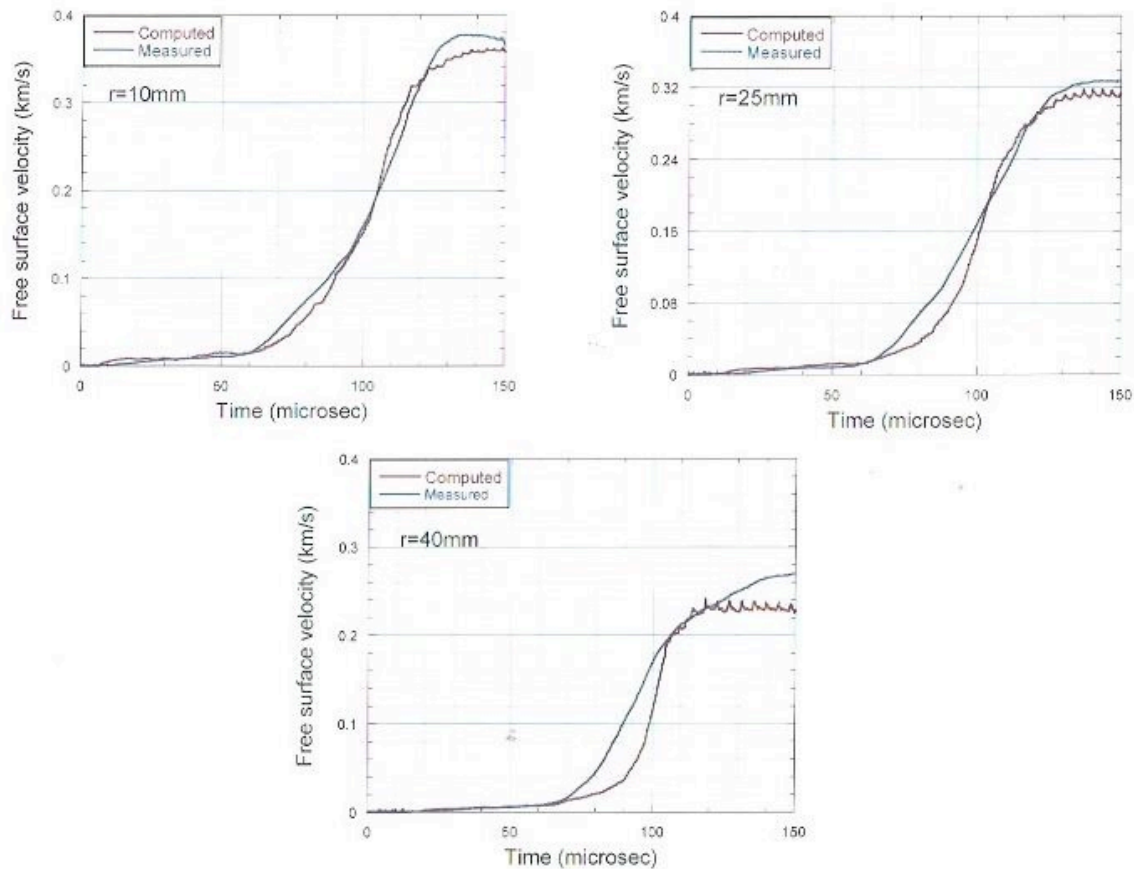


Figure 7. Comparison of measured results from Fig. 5 and computed results from Fig. 6. Each sub figure is for a different radial distance.

We see from Figs. 5, 6 and 7 that the agreement between test results and computations is not perfect but quite reasonable. As explained above, the agreement may be considered reasonable because we're dealing with a safety problem.

Finally, we're showing in Fig. 8 the above computation results by means of maps with lines of equal W . From those maps we see that: 1) almost all the explosive has reacted, at least partially; 2) the front plate was broken through, and 3) the back plate and the radial ring deformed plastically, but stayed intact.

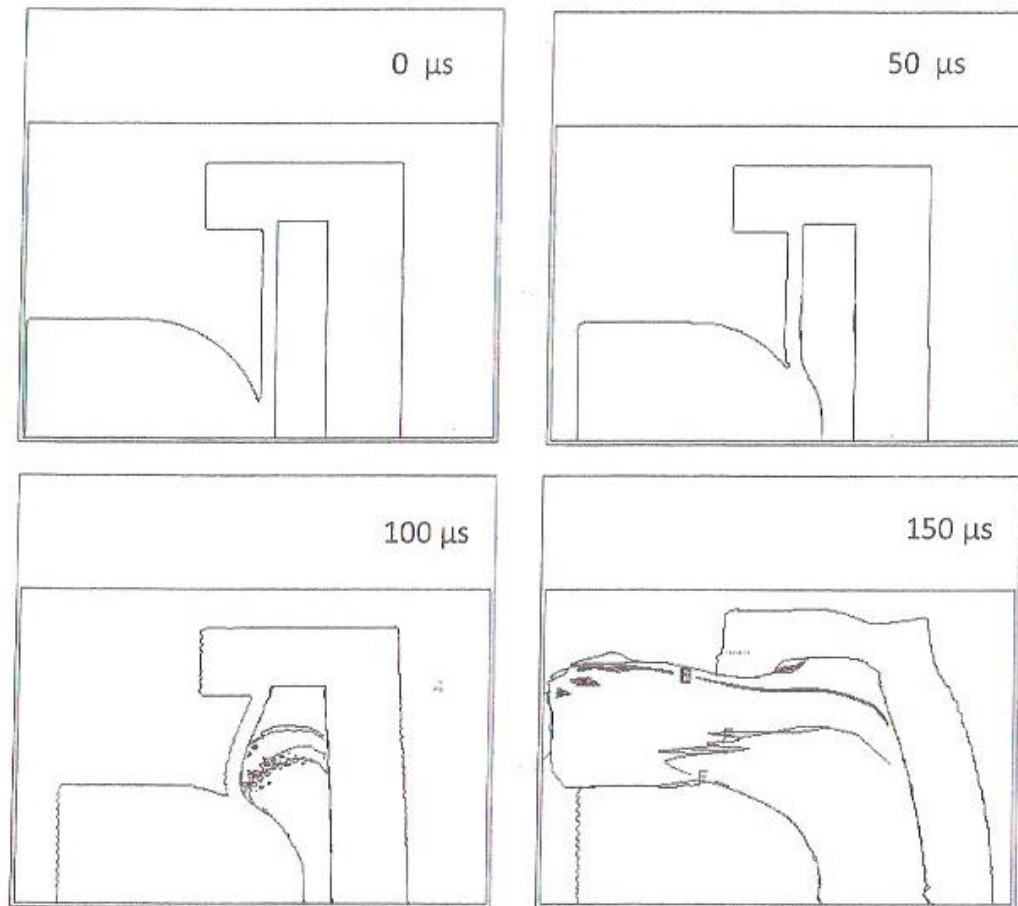


Figure 8. Maps with lines of equal W from computations for an impact velocity of 120 m/s, at times 0, 50, 100 and 150 μ s.

Shear reaction of propellants

Propellants are “weak” energetic materials compared to explosives. Regular propellants usually contain three types of materials: a “weak” explosive like ammonium perchlorate, aluminum powder, and a plastic binder. “strong” propellants may contain a strong explosive like RDX or HMX.

Performance of a propellant in a rocket engine is characterized by its burn velocity and by its burn stability under different conditions. Rocket engine developers are therefore well acquainted with the burn properties of propellants. But propellants, because they contain explosives, may also explode, or even detonate. As explosion and detonation of propellants are unusual events, they are related to safety aspects of rocket engines, and not to their performance. And because usually, knowledge on safety aspects is less common than on performance, such is also the situation with respect to explosion and detonation of propellants. There is however an additional reason to the relative lack of knowledge on explosion and detonation of propellants. The reaction rate of explosives is high, it's therefore possible to characterize their detonation properties with relatively small samples, of the order of 1-100mm. In contrast, reaction rate of propellants is rather low, and to characterize their

explosion and detonation properties we need to use quite sizable test bodies. One way to demonstrate this difference between propellants and explosives is by means of the property known as critical diameter. The critical diameter of PBX9501 is 2.5mm. It's therefore possible to characterize the detonation properties of this explosive with tests on samples smaller than 100mm. In contrast, the critical diameter of regular propellants is of the order of 1m and more. To characterize their detonation properties, we therefore need huge samples with size of several meters. Such tests are prohibitive to perform, which is why there is little knowledge on detonation properties of propellants.

Safety considerations of rocket engines are usually related to their storage and handling. Usually, rocket engines are stored in concrete bunkers. To design such a bunker, one needs to estimate the internal loading on the bunker structure caused by the explosion or detonation of the stored propellant of the rocket engine. To this end it is customary to represent the amount of propellant in the bunker in terms of a representative amount of explosive. The coefficient of such a representation is called "Explosive equivalent" or, what is more common, "TNT equivalent" (TNTE). For TNTE=1 the bunker designer computes the structure loading as if the mass of TNT exploding in it is equal to the mass of propellant stored in it. As explained above, the TNTE values for common propellants are not really known, and one finds in the literature contradicting values for them. This is why rocket engines storage bunkers are usually designed with TNTE=1, which is probably an over-design.

With one of our projects, we have to build storage bunkers for very large rocket engines. Assuming TNTE=1 would lead to expenses we can't afford, and we decided to conduct a small research program, to see what we really need to assume as a realistic loading of the bunker structure, in case that such an engine reacts.

We conducted several not too large tests of the following configuration. A propellant cylinder 125mm in diameter and 500mm long. The cylinder is encased in an aluminum shell 5mm thick. On one side of the cylinder (left in Fig. 9) we detonate an explosive charge (PBX9501). We use velocity gauges to measure the radial velocity history of the aluminum shell at several distances from the left boundary. We expect a strong reaction to start near the detonating explosive, that would continuously decline, as the reaction wave moves to the right. This is because the cylinder diameter is much smaller than the propellant critical diameter. The reaction wave in the cylinder would be reflected in what the velocity gauges measure. So finally, being able to reproduce the gauge signals with our computer simulation would establish the validity of our propellant reaction model, and make it possible to use it to predict the response of other propellant loading configurations.

In Fig. 9 we show a schematic plot of the test configuration.

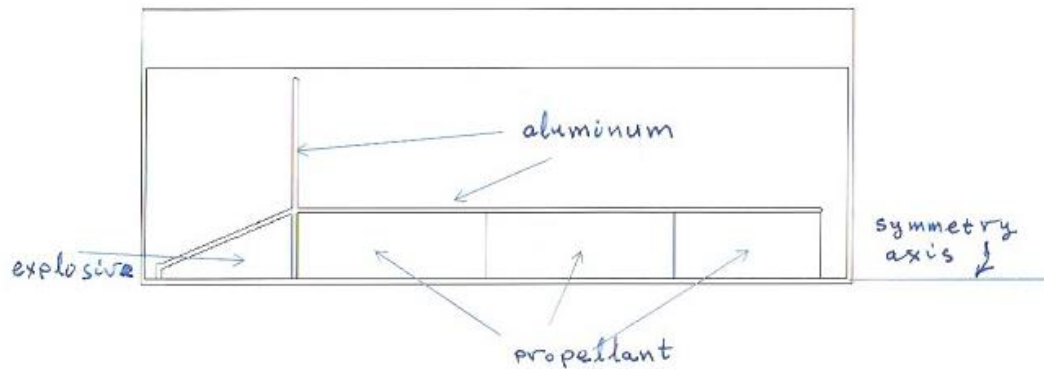


Figure 9. Schematic plot of the test configuration. The explosive is initiated on the axis on the left side. The aluminum skirt stops fragments and gasses to reach the gauges. The radial velocity gauges are at distances of 30,70,110,150,250,350 and 450mm from the propellant left boundary

In Fig. 10 we show results of a test described in Fig. 9.

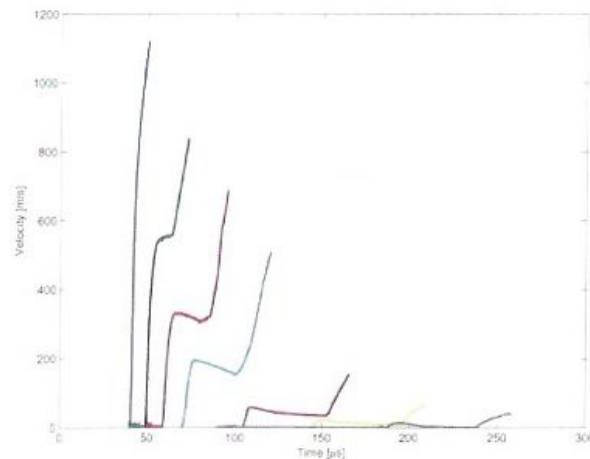


Figure 10. Histories of the radial velocities of the aluminum outer boundary as measured by the 7 gauges of Fig. 9

From the gauge traces of Fig. 10 we see that: 1) the first jump level of gauges 2 to 7 decreases with distance along the propellant cylinder; 2) comparing to a reference test where the propellant was replaced by an inert material of the same density (not shown), we see that the first gauge signal is almost the same; 3) there is a delay of 0 to $50\mu\text{s}$ between the first jump and the second jump; 4) there is a second velocity increase before the signal is cutoff. We're not able to explain this cutoff, but we're sure it results from the specific layout of the gauges. The delays we get in the signals of Fig. 10 are reminiscent of what we discussed in the previous chapter in relation to shear reaction of explosives, but here the amount of delay is changing. Accordingly, we assume that the amount of delay decreases with temperature. In the simulations we therefore assume that a deflagration wave that decays with distance (and not a detonation wave) propagates through the propellant. We use the same reaction equation that we used in our TDSR model in the previous chapter, but with the following coefficients:

$$\begin{aligned} (PD)_{\text{ign}} &= 0.02 \text{ GPa}/\mu\text{s} \\ R_{\text{SB}} &= 0.1 \text{ GPa}/\mu\text{s} \end{aligned} \quad (3)$$

We see that for propellants ignition threshold is higher than for explosives, but the reaction rate coefficient is lower by a factor of 250, and this difference expresses the fact that propellants are by far less reactive than explosives.

In Fig. 11 we show maps of sections through the test body with lines of equal reaction parameter, every 40 μs .

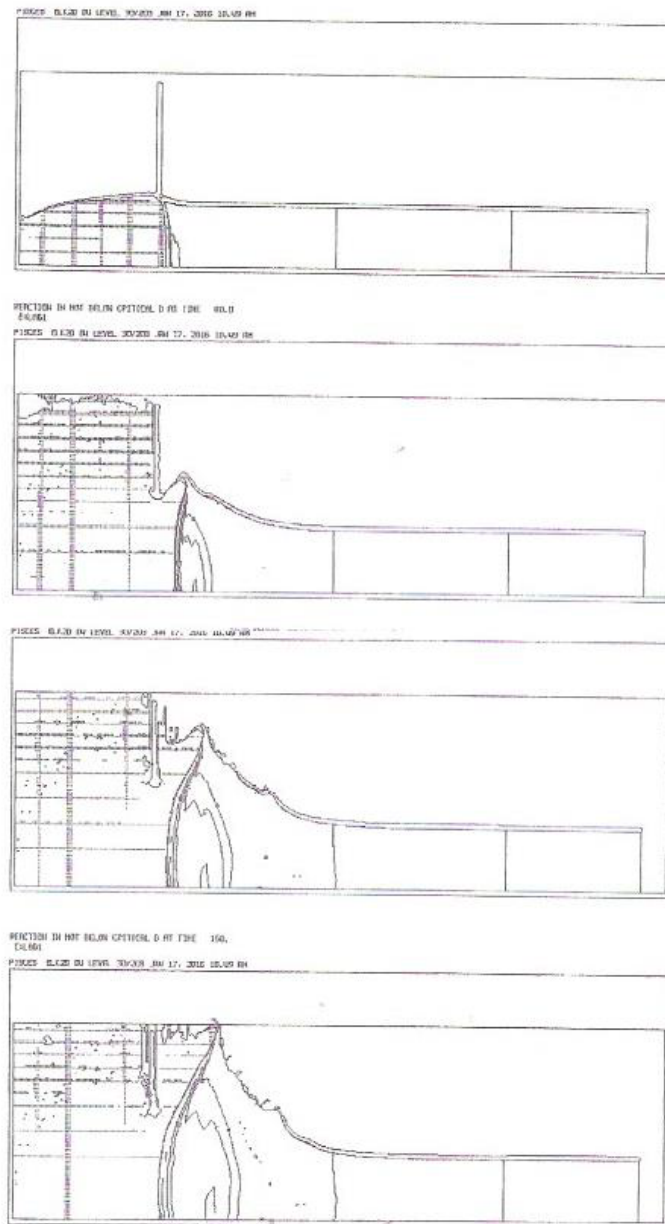


Figure 11. Maps with equal reaction parameter lines from the simulations, at times of 40,80,120 and 150 μs

In Fig. 12 we show the particle velocity signal of gauge 2 (70mm along the propellant) from our simulation.

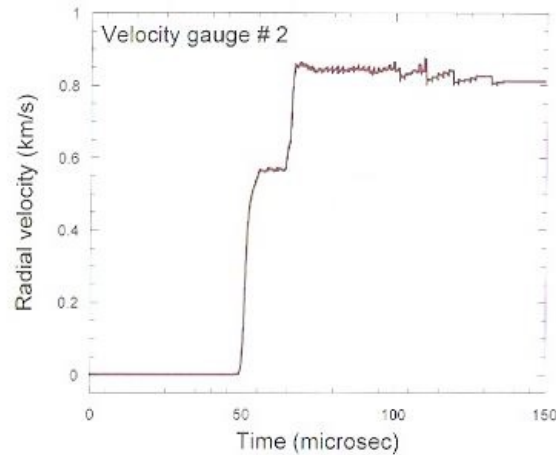


Figure 12. Radial velocity history of gauge 2 from our simulation

From Fig. 12 we see that: 1) after 50 μ s a velocity jump is obtained similar to the test result; 2) 15 μ s later, the radial velocity starts to decrease slowly.

In Fig. 13 we show the radial velocity signals of the first 5 gauges, as obtained from the simulation. To make these signals resemble the test signals, we omitted from them the upper almost horizontal part.

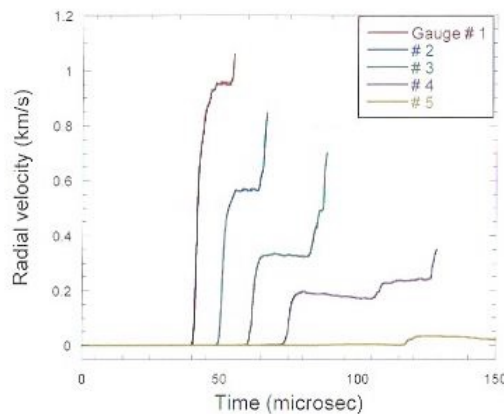


Figure 13. Radial velocity histories of gauges 1 to 5 as obtained from the simulation. The top part of the curves was cut off, to make them look like the experimental signals

Comparing Fig. 13 to Fig. 10 we see that generally there is a resemblance between corresponding curves in the two plots.

In Fig. 14 we show simulation results where we increased the coefficient of the reaction rate equation by a factor of 10. We see from Fig. 14 that the propellant was made to respond much like an explosive. We also performed a test with the propellant replaced by an explosive (the results of which we don't show here), and the velocity signals we got are much like those of Fig. 14. We may conclude from this that an essential difference in the response of propellants and explosives to shear loading is related to the magnitude of their reaction rates.

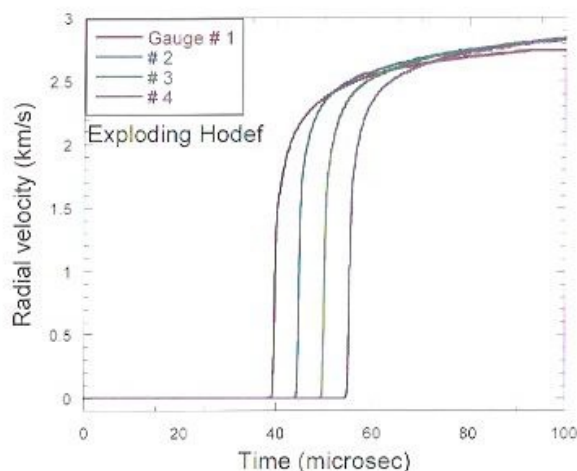


Figure 14. Radial velocity histories of the first 4 gauges, with the reaction rate coefficient increased by a factor of 10

SUMMARY

In the introduction we review different forms of ignition and reaction of energetic materials under impact. Here we deal with the response of energetic materials (explosives and propellants) to weak impact, which has mainly to do with safety aspects. A weak impact may ignite an energetic material through the formation of shear bands, which heat up to the ignition temperature by a process that is relatively slow (takes about 50 μ s). We refer to such a process as shear initiation, and we represent it in our hydrocode by a simulation model that we call TDSR (= Temperature Dependent Shear Reaction). To demonstrate shear reaction of an explosive we use the well-known Steven test with improved diagnostics. To demonstrate shear reaction of a propellant we use our own test configuration. It consists of a long (500mm) cylindrical sample covered by a 5mm aluminum layer, impacted on one end by a small explosive charge. The diagnostics include radial velocity gauges that measure the radial motion of the aluminum layer at several longitudinal locations. We simulate both tests with hydrocode simulations where we use our TDSR reactive flow model, and find reasonable agreement to test data.

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