UR-79-3106



CONF-790975--4

PRIMER ON SDT, DDT, XDT, PICKUP, AND SYMPATHETIC TITLE: DETONATION

Louis C. Smith AUTHOR(S): Bobby G. Craig

SUBMITTED TO:

16th JANNAF Combustion Meeting September 10-14, 1979 Naval Postgraduate School, Monterey, CA

- DIECLAMER

O state program is an account of states destination by an approximate of the Entreet States destination of the approximate of the entreet states and approximate of the entreet state and of the approximation of the end of th naanto dage oo ing booglag. Meel af of af of generations o na paga na paga paga paga na paga na paga paga paga na paga na paga paga paga paga

By acceptance of this article, the publisher recognizes that the U.S. Government retains a nonexclusive, royalty-free license to publish or reproduce the published form of this contribution, or to allow others to do so, for U.S. Government purposes.

The Los Alamos Scientific Laboratory requests that the publisher identify this articl as work performed under the auspices of the U.S. Department of Energy.

LOS ALAMOS SCIENTIFIC LABORATORY

Post Office Box 1663 Los Alamos, New Mexico 87545 An Atlimative Action/Equal Opportunity Employer



Form No. 836 R3 St. No. 2629 12/78

University of California

UNITED STATES DEPARTMENT OF ENERGY CONTRACT W-7408-ENG. 34

PRIMER ON SDT, DDT, XDT, PICKUP, AND SYMPATHETIC DETONATION*

Louis C. Smith and Bobby G. Craig University of California, Ios Alamos Scientific Laboratory, Los Alamos, New Mexico 87545

When Bob Craig asked me to give this talk, what I agreed to was to present an elementary discussion of DDT and SDT. When I received the printed program I was surprised to discover that my assignment had broadened considerably. Fortunately, time will come to my rescue. There is only so much one can say in thirty minutes, especially about a topic we don't know much about anyway. Besides, I only have to get the ball rolling; various aspects of the subject will be covered in detail in other papers to follow.

The C-4 movie shown by LeRoy Throckmorton presents a spectacular example of a chain of events that underlies essentially all accidental detonations. The chain, in a reasonably complete form, is shown in Fig. 1. We can enter the chain -- that is, an accident can start -- at any one of the boxes.



FIG. 1. THE DDT CHAIN,

I will first describe the chain qualitatively, proceeding from left to right because that's the way things happen in real life. I will then try to summarize what we know about the individual links in the chain. For that I will take them in reverse order because our knowledge decreases rapidly as we go from right to left.

We start with two events, charge breakup and ignition, that may occur simultaneously or in either order. What is required is that we obtain rapid ignition of a sufficiently large surface to support the rest of the process.

"Sponsored by the U.S Deportment of Energy, Contract W-7405-ENG. 36. Approved for public release; distribution unlimited. The word in the next box, deflagration, means different things to different people. To me, in this context, it implies a rapid and rapidly accelerating combustion process. The deflagration must result in the formation of a shock wave somewhere in the system. If the shock is sufficiently intense and conditions are otherwise favorable, a shock-to-detonation transition (SDT) will occur and the entire charge will be consumed in a matter of microseconds. The last three boxes together form a deflagration-to-detonation transition (DDT).

Let us now retrace our steps and discuss the various elements in the chain in greater detail. Much of what I will say is controversial or speculative, so if the person next to you snickers at my way of explaining something, it's probably because he thinks he could do it better - and maybe he could.

This talk is supposed to be a primer, so before I discuss SDT I will say just a few words about detonations in condensed explosives. A detonation wave is an intense, reactive shock wave which travels through the explosive at a velocity typically in the range of 5000 to 9000 m/s - some two to three times the longitudinal sound velocity in the unreacted material. The front of the shock compresses the cold explosive, heating it to a temperature such that it decomposes in a microsecond or less. In decomposing, the explosive releases some 1000 to 1500 cal/g of energy and a large volume of gas, about a liter per gram, which serves as the working fluid when the products do work on their surroundings. At the completion of reaction, at what is called the Chapman-Jouguet or C-J point, the temperature is about 3000 K and the pressure several hundred kilobars. The detonation velocity usually increases linearly with density with a slope of around 3200 m/s for each g/cm^3 increase in density. The detonation pressure increases approximately as the square of the charge density, which is why high density is important in some applications of explosives.

Obviously, not all shock waves that travel through an explosive charge are detonation waves. More generally, the nonreactive shock waves in any material define what is called the Hugoniot of the material. Hugoniots frequently take the form

 $U_s = C_o + SU_p$

where U_S is shock velocity, C_O is the bulk sound velocity, S is a coefficient, and U_D is the particle velocity associated with the shock (the particles acquire kinetic energy when a shock wave passes through). However, Hugoniots are not always linear in the U_S-U_D plane. They may curve gently, or they may exhibit abrupt changes in slope. The latter usually signifies that a phase change has occurred.

Hugoniots are determined experimentally; Jerry Dick will describe one way of doing so in his paper on the wedge test to

Ĩ.

be given tomorrow afternoon.* Used with relations derived from the conservation of mass, momentum, and energy, the Hugoniot provides a description of the hydrodynamic and thermodynamic state of the explosive behind a shock wave (an equation of state is also needed for a complete description).

Some shock waves may cause incomplete reaction of the explosive. Except in rare cases, this represents an unstable situation. If the shock is intense enough, it will accelerate (build up) and become a detonation. Otherwise it will decay and fade away. A very useful approximation that works in many situations is called the single-curve buildup hypothesis.² It relates pressure and distance of run, as shown in Fig. 2. The hypothesis states that the buildup process will follow this curve, from left to right, no matter where on the curve the process starts.

An actual example is shown in Fig. 3. This is a plot of data from four experiments on FKM. The origin of the time axis is the time at which detonation occurs. The solid symbol in each case gives U_S and t for the entering shock for that experiment; the remaining symbols of each type then describe the buildup of that shock. There is evidence in this example of a





[&]quot;In the absence of experimental data, the Hugoniot of an organic explosive can be estimated from its molecular structure and density by means of a generalized Hugoniot. See, for example, Ref. 1.



FIG. 3. TEST OF SINGLE-CURVE BUILDUP HYPOTHESIS FOR FKM.

slight departure from the single-curve hypothesis; the squares lie slightly above the circles, the triangles above the squares, etc. The agreement is usually better, but I used this example because it was readily available in the form I needed.

Another useful relationship connects x^* , the buildup or run-up distance, with P_0 , the pressure in the entering shock wave. This relationship is commonly called the Pop Plot after Al Popolato, one of its discoverers.³ It takes the form

 $x^* = bP_0^a$

so that Pop Plots are straight lines on log-log paper. From the Pop Plot and the single-curve buildup hypothesis it is possible to back out the decomposition rate as a function of the local thermodynamic state of the explosive. One procedure for doing this is known as Forest Fire after Charles Forest, its inventor.⁴

The Pop Plot, which is also determined experimentally, is central in the SDT process. To see why this is so in a very simple case, let us refer to Fig. 4. A projectile strikes a cylinder of explosive of radius r at the left, sending a shock wave of pressure P_0 into the explosive.* Initially the whole cross section of the cylinder is at pressure P_0 , but as soon as the wave starts down the stick, a rarefaction wave travels radially inward with the local velocity of sound, relieving the pressure. Thus the area compressed diminishes steadily as the wave proceeds into the charge, as shown by the dotted line, and the wave essentially vanishes at a distance approximately equal to rU_S/C . If x* for this pressure is greater than rU_S/C , detonation will not occur.** Pop Plots for several explosives and propellants are shown in Fig. 5. The one for FKM, for example, tells us that a plane, flat-topped, 40-kbar shock in FKM will build up to detonation in about 10 mm of run.

What's going on in the explosive while buildup is occurring? That is, where does the energy come from that causes SDT? The temperature behind a 40-kbar shock will be about 170°C, far too low for ordinary thermal decomposition to be significant. The most likely source of chemical reaction

"Note that the pressure of the shock wave in the explosive depends on the velocity of the projectile and the Hugoniots of the projectile and target - which is one reason it is important to know the Hugoniots.

**For shocks near the "critical" pressure detonation also will not occur if the diameter of the shock becomes less than the failure diameter of the explosive.





(energy) appears to be a hot-spot/combustion process. Voids and density discontinuities perturb the shock and produce microscopic regions of very high temperature and pressure in which decomposition is almost instantaneous. These small regions then burn outward. As the pressure increases the burning rate increases, and initially the burning area also, so that the process is an accelerating one. Eventually the temperature may become high enough for thermal decomposition to occur also. If conditions are right, the wave ultimately becomes a detonation wave.

The question is, Is this model plausible? In Table I I have listed a set of conditions that would suffice for a 20kbar shock in PBX 9404 (94/3/3 - HMX/NC/CEF). The decomposition rate, λ , is obtained from the Forest Fire rate law. The burning rate, r, is obtained by extrapolating data obtained on HMX at lower pressures. The burning area follows from λ and I have taken 7 μ m for the hot spot radius for reasons I will mention shortly; too large or too small a value leads to unreasonable results. I can then calculate the number of hot spots/cm³ required to give the necessary combustion rate. If I assume that the HMX particles are uniform $60-\mu m$ spheres, I have 2.6 hot spots per HMX crystal; somewhere around 1 or 2 would seem about right, so that's not too bad. If they were distributed uniformly on a cubic lattice the hot spots would be 35 µm apart, center to center. The hot spots occupy 3.3% of the volume of the explosive. From data by Ramsay and calculations by Mader² I estimate 3% uncomposition behind a 20 kbar shock in PBX 9404. It was for that reason that I chose 7 µm for the hot-spor radius (the hot-spot volume is proportional to the assumed radius).

The last line of the table is an estimate of flame thickness derived from information provided by Chan Price of NWC. Most people ignore this factor in discussing the com-



FIG. 5. PUP PLOTS (DENSITIES IN G/CM³ GIVEN IN PARENTHESES).

TABLE 1. A Hot-Spot Model for PBX 9404.

 $\lambda = 0.02/\mu s$ r (20 kbar, 100°C) = 1.4 x 10⁻⁴ cm/ μs Burning area = 140 cm² Hot-spot radius (assumed) = 7 μm No. of hot spots/cm³ = 2.3 x 10⁷ No. of hot spots/60- μm HMX crystal = 2.6 Hot-spot separation, center to center (ave) = 35 μm Hot-spot volume/cm³ = 0.033 cm³ Hot-spot energy = 85 cal/cm³ Flame thickness (est) = 0.5 μm

bustion model, but it seems evident to me that, for a flame to exist in a hot spot, the flame thickness must be less than the hot-spot radius. There seems to be no problem with this example. However, it is tempting to speculate that the reason certain explosives, such as NQ and TATB, are so insensitive to shocks is because their flame thickness is always too large, so that this model cannot provide the necessary growth. Shock initiation will then depend on thermal decomposition, and this in turn will require much higher shock pressures.

One can quibble with the manner in which I have constructed Table I, but my own conclusion is that for most explosives the hot-spot/combustion model will provide the observed decomposition rates with credible values of the various physical quantities. Note that this model applies only to nonhomogeneous explosives; liquids and single crystals conform to a quite different model.⁵

I have now discussed the last box in Fig. 1, having described both the qualitative features of SDT and a model that seems to work. Proceeding to the left, we come to the one labeled shock formation. Our problem here is to explain in a physically plausible way how a combustion can lead to the formation of a shock of some tens of kilobars. Obviously, combustion under heavy confinement can lead to very high pressures, but uniform high pressure is not a shock wave. What is required is a sufficiently high rate of rise in the pressure.

In discussing this, nearly everyone sooner or later gets around to drawing something like Fig. 6. At the left we start out with a ramp wave, with a steep pressure gradient. Sound velocity increases with pressure, so that the higher pressure parts of the wave travel faster than the lower pressure parts. The result is that after some distance (or time) the wave steepens and becomes a shock, as shown at the right. The shock must form before a signal can get back from a free surface or before the wave reaches a free surface. Otherwise, the pres-



FIG. 6. SHOCK FORMATION FROM A RAMP WAVE.

sure is relieved and a shock never forms. We can thus see in a qualitative way that:

a) The steeper the gradient, the more rapidly the shock will form.
b) The time available for shock formation increases with the size of the system.

Not so obvious, perhaps, is that to reach the pressures required we usually have to depend on the inertia of the system to provide the necessary confinement.

It is beyond the scope of this paper to discuss analytically how steep the pressure gradient must be. Qualitatively it would seem as though kilobars in microseconds must be the order of magnitude required.

As was already noted, to attain the pressures and pressure gradients required for SDT requires a rapid and rapidly accelerating combustion process - called Deflagration in Fig. 1. The necessary rapidity can be obtained by having a high enough burning rate and a large enough burning surface in a sufficiently small volume. The acceleration can be obtained in several ways, but the increase with pressure provided by the usual burning law, cPⁿ, is usually adequate.

Many DDT problems in one and two dimensions can be calculated numerically given the properties of the explosive, the geometry of the system, and the combustion area as a function of time. An example calculated by Forest is shown in Fig. 7. This is a one-dimensional problem in cylindrical geometry, chosen because it illustrates some of the more interesting features of the DDT process. Initially we have a porous bed of





propellant in the form of an annulus 2.0 cm thick at 90% of TMD. Outside the annulus is an aluminum case, inside is a solid grain. The surface-to-volume ratio in the porous bed is 75/cm; the bed is assumed to consist of uniform spherical granules. It is further assumed that at t = 0 the entire surface of the porous bed is ignited simultaneously and that the pressure in the bed is 760 atm. The burning law used is 0.00773 $p^{0.942}$ cm/µs with P in megabars. A Forest Fire rate law is used for the solid grain. The top half of each frame gives the mass fraction of propellant remaining. The lower gives the pressure as a function of position; the scale varies as shown in the lower right-hand corner. The time in micros-conds is given in the lower left-hand corner.

In the first frame, at 10 μ s, a ramp wave is moving into the solid grain. At 40 μ s the maximum pressure is about 14 kbar, and we're beginning to see some decomposition in the solid grain. At 50 μ s the maximum pressure is over 50 kbar and the wave has steepened into a shock. Note that decomposition in the grain is now occurring mostly at the shock front. At 51.7 μ s detonation occurs at a radius of about 9.5 cm. Decomposition in the porous bed is still only 20% complete.

In cylindrical geometry convergence of the wave may be very important in the buildup process. In fact, in 1-D calculations such as this detonation will always occur in a solid grain. Real motors, of course, have center bores, so the calculations are more meaningful for such cases.

A much more difficult problem is that of calculating the rate at which the flame penetrates a porous bed; we sidestepped that in the example above. I expect we will hear something about this this afternoon in the paper by Hopkins et al. These are certainly noble efforts, but I sometimes wonder if it will ever be possible to include all the physics - such as the effect of turbulence in the hot gas, for example.

We are left with the two boxes at the extreme left of Fig. 1. As we have seen, breakup of the charge is needed in order to obtain a high enough surface-to-volume ratio for the next step in the chain. Breakup of the degree required usually occurs by impact or shear. Materials scientists are trying to treat these processes analytically, but they have a very tough row to hoe! As to ignition, it may already be present, as in LeRoy's examples, or it may be provided by any one of a number of processes that produce a local concentration of heat. Although superficially the concepts seem simple enough, ignition and flame-spreading again pose some difficult analytical problems. In the case of ignition of a solid by a hot gas, for example, surface roughness may be of paramount importance.⁶ We'll hear more about these matters tomorrow morning. As I suspected, my time is almost up and I still haven't gotten to XDT, pickup, and sympathatic detonation. I have told you much of what you will need to know to understand the qualitative features of these processes, however, and all will be covered in talks to be given later on today. I will make a few comments regarding how these processes are related to my Fig. 1.

In the simplest case of sympathetic detonation, not involving fragments, we enter the chain at the penultimate box. The air shock and the motion of the detonation products from the donor charge establish a ramp wave in the acceptor charge. The ramp quickly becomes a shock, and SDT follows. Problems of this sort are susceptible to numerical analysis, as Al Bowman will tell us 'his afternoon.

Sympathetic detonation by fragments is another matter entirely except for certain special cases that can be treated as one- or two-dimensional SDT problems. The more usual cases require two- or three-dimensional treatments of the entire chain, starting with charge breakup and ignition by friction or viscous flow. Needless to say, the empirical approach predominates here.

XDT and pickup are newly coined terms. So far as I know, XDT doesn't have a generally accepted definition. It is understood to represent a process similar to SDT, but which occurs on a longer time scale - after first passage of the initial shock wave. It might also be a very rapid DDT. Pickup usually refers to experiments in which one piece of propellant, fired from a gun, strikes a second piece located a short distance frcm a target plate. The second piece is damaged by the impact, and both pieces then strike the target plate. The purpose is to determine whether DDT occurs more readily in freshly damaged propellant. These two phenomena presumably enter the chain at Charge Breakup and then proceed through Ignition on to Deflagration. I believe we will hear about both later on this morning.

REFERENCES

- A. N. Afanasenkov, V. M. Bogomolov, and I. M. Voskoboinikov, "Critical Initiation Pressures of Explosives;" in "Control of Noxious Gases in Blasting Work, and New Methods of Testing Industrial Explosives," B. D. Rossi, Ed. Translation available from U.S. Department of Commerce, National Technical Information Service, Springfield, VA 22151.
- C. L. Mader, "The Two-Dimensional Hydrodynamic Hot Spot, Vol II," Appendix D. Los Alamos Scientific Laboratory report LA-3235 (1964).

- 3. J. B. Ramsay and A. Popolato, "Analysis of Shock Wave and Initiation Data for Solid Explosives;" in "Proceedings of the Fourth Symposium (International) on Detonation."
- 4. C. L. Mader and C. A. Forest, "Two-Dimensional Homogeneous and Heterogeneous Detonation Wave Propagation." Los Alamos Scientific Laboratory report LA-6259 (1976).
- 5. A. W. Campbell, W. C. Davis, and J. R. Travis, "Shock Initiation of Detonation in Liquid Explosives." Phys Fluids <u>4</u>, 498 (1961).
- 6. E. E. Kiselev, A. D. Margolin, and P. F. Pokhil, "Shock Ignition of Po.ders." Fiz Goreniya i Vzryva <u>1(4)</u>, 83 (1965).

.