Conf-9409195--1

LA-UR- 94-2837

Title: FRONTIERS OF DETONATION THEORY

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Submitted to: Microscopic and Macroscopic Approaches to Detonation
St. Malo, France
September 2-7, 1994

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PART 4

FRONTIERS OF DETONATION THEORY

William C. Davis

Abstract

Detonation theory is far from complete for many reasons. As one example, although it can be used to predict performance of explosives, it does not serve to predict effective reaction zone lengths. The flow is not smooth and laminar, but violently multi-dimensional on a small scale, and small hot spots produced by the flow localize the initial part of the chemical reaction, and influence its evolution. The present inability to model these phenomena not only prevents needed predictions, but also prevents the use of detonation experiments for studying chemistry in a region of state space not attainable in the usual laboratory. The underlying difficulty in these and other cases where the mechanics and the chemistry interact arises because of the large number of disparate space and time scales in detonation problems.

All detonation studies involve the interaction of chemistry and mechanics. In the detonation reaction zone the flow is not smooth and laminar, and consequently the shock wave is not smooth. The result is that the explosive is not heated uniformly, and the chemical reaction rate, an extremely non-linear function of temperature, is much more non-uniform. Reaction is fast in some small regions, usually called hot spots, and, relatively, almost nonexistent elsewhere until it spreads from the hot spots.

In cast solid explosives, pressed polycrystalline explosives, emulsions and slurries, and in loosely packed powders, most of the hot spots are in the neighborhood of lower density regions. Where the density is low, the motion is greater, and more work is done on the material by the motion. The internal energy rises there, and the temperature is higher. The scale of the hot spots is related to the size of the crystallites or the rate of cooling when casting, etc., and these sizes are determined by such considerations as convenience for handling. How much reaction takes place at a hot spot depends of the rate of reaction and the rate of diffusion of heat away from the hot spot. In two explosives with crystallites the same size but reaction rates very different, the apparent effect of the hot spots may be very different.

In liquid explosives, it might seem that there will be no hot spots. Nature is not so kind. The flow in a detonation in a liquid explosive is still not smooth and laminar, because the burning is hydrodynamically unstable[1], and generates transverse waves spontaneously. (The solid explosives discussed in the preceeding paragraph also have these instabilites, and they compete with the ones generated by inhomogeneity.) The scale and the spacing of these hot spots is related to the scale of the chemical reaction zone; the details are not understood, and are a subject for future research. The structures that have been studied seem to have a spacing of a few, 3 to 10, reaction zone lengths.

Detonation in gases[2] produces very strong transverse waves, often with a shock wave collision called a Mach stem, where the pressure and temperature are far above the average. In some cases almost half the gas flows through this interaction region. It is as if the detonation, unable to propagate in a laminar flow, created superchargers for itself to ensure propagation. Gas detonations have been studied extensively (they do not destroy the equipment, the equations of state are known, the flow is transparent, and the transverse wave structures can be made large by reducing the initial pressure) and much is known about the details of the transverse waves. It is tempting to believe that structures in condensed phase explosives are analogous to those in gases. After all, if one explosive is not more like another explosive than anything else, there can be no science of explosives. But probably gases are different from liquids and solids. The spacings are 100 or more reaction zone lengths. The mechanical details are very different because of the differences in the equations of state.

The published papers[2] on detonation abound with papers on hot spots. It has been known for a very long time that imperfections and inhomogeneities strongly influence the critical size below which detonation will not propagate, and that many explosives must have hot spots to be useful. Two batches of explosive with identical chemical composition may differ enough in their hot spot behavior to make one batch useful and the other useless. Obviously, producers of explosives have learned to control the hot spots. The knowledge is all empirical.

One result of the current inability to model the effects of all the varied phenomena lumped together under the heading hot spots is that there is no way to take any available knowledge of chemical reaction rates for well-defined chemical explosive and predict what a particular formulation will do. For example, in one long list comparing the sensitivity of explosives in the gap test, a cast TNT formulation was the least sensitive explosive, and a pressed TNT formulation was the most sensitive. When the behavior of the explosive is accurately described by the simple classical theory discussed in Parts 1&2 of this introduction, that is, when the effective reaction zone length is small relative to system dimensions, the reaction rate has little effect on performance. Part 3 made it clear that safer explosives with long reaction zones cannot be described so simply, and the details of the phenomena in the reaction zone are important. When transient behavior is important, as in initiation of detonation intentionally, and even more in accidental initiation, the reaction zone in all its multi-dimensional detail, is even more important.

The difference between the classical theory of Parts 1&2, and the more complex ideas of Part 3&4, is that the classical model has only one important space scale, the reaction zone length. In most of Part 3 the dimensions of the charge provide another space scale. Above in Part 4 a scale of inhomogeneity was added. There are many space scales that are important in some detonation problems; fortunately not all of them are important in all detonation problems. When the flow is steady or nearly steady, that is, a wave moves but changes only slowly with time, space and time scales are simply related. When the transients are considered, space and time scales are not so neatly interchangeable.

A list of some important space scales is given in Table I. It is just an evaluation of the order of magnitude of these scales, and is arbitrary in many respects. However, it shows an enormous range. Modeling, whether analytical or computational, for systems where the ratio of important space scales is large presents great difficulties.

New developments in detonation theory are needed to incorporate treatments of all the important processes at their disparate scales. The new approaches discussed in Part 3 are a start. This meeting, with its title "Microscopic and Macroscopic Approaches to Detonation", is directed to the frontiers of detonation science.

TABLE I

Item	Scale (meter)
charge size	10^{-1}
reaction zone length	$10^{-5} - 10^{-2}$
crystallites, dendrites, emulsions	$10^{-5} - 10^{-3}$
hot spots	$10^{-7} - 10^{-4}$
shock roughness	$10^{-7} - 10^{-4}$
shock thickness	10^{-8}
atoms and molecules	10^{-10}

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2. S. L. Crane, W. E. Deal, J. B. Ramsay, A. M. Roach, and B. E. Takala, Index for the proceedings of the Symposia (International) on Detonation, 1951-1989. Tenth Symposium (International) on Detonation, preprints p. 473, 1993. There are 75 entries under the heading "hot spots".