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The physics, chemistry and dynamics of explosions

Elaine S. Oran and Forman A. Williams

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Introduction

The physics, chemistry and dynamics of explosions

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The motivation for devoting a Theme Issue to explosions is discussed. As subsequent articles in the issue are written with the assumption that the reader has had a certain amount of previous exposure to the subject, some of the history and necessary background information are presented here. The topics on explosions that will be encountered in the remaining articles are previewed. Finally, several important future outstanding research problems, beyond those addressed in the following articles, are discussed, with the objective of complementing the coverage of explosions in this issue.

Keywords: explosion; detonation; deflagration; deflagration-to-detonation transition; turbulent reacting flows; astrophysical explosions

1. Introduction

Explosions are ubiquitous in the Universe. Beginning with the Big Bang, the history of the Universe has been determined largely by explosions, which disrupt orderly progression and initiate evolution in new directions. While intergalactic and galactic explosions are of many different types, explosions on the Earth involve a narrower range of phenomena that are somewhat more amenable to human understanding. Effects of explosions on humankind, both beneficial and detrimental, have been investigated from the beginning of science, resulting today in a degree of knowledge of their properties—their physics, chemistry and dynamics. During the past century, this knowledge has been used both to design explosions for specific purposes and to teach us how to avoid those that are harmful. Any knowledge, however, can be used or misused, for actual or misconceived benefit. Possible future advances include mitigation of explosion hazards, improved and new combustion engines and use of inertial confinement for the development of nuclear fusion as an energy source.

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One contribution of 12 to a Theme Issue 'The physics, chemistry and dynamics of explosions'.

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The term explosion itself is nebulous. It generally refers to any type of scenario in which energy is injected into a system faster than it can be smoothly equilibrated through the system; that is, energy is deposited faster than a dynamical time scale. For chemical or nuclear explosions, this time scale (l/c_s) is based on the characteristic size (l) of the system and the acoustic velocity (c_s). For magnetohydrodynamic explosions, c_s is replaced by the square root of the sum of c_s^2 and the magnetoacoustic time scale c_{ma}^2, where c_{ma} is proportional to the speed of Alfven waves, the square of which, in turn, is proportional to the magnetic pressure. The result of this rapid injection of energy is a local pressure increase. If the system is unconfined, or if the confinement is weak and can be broken, then strong pressure waves (shock waves) develop and spread outwards, travelling considerable distances before they are dissipated. As this happens, over-pressurized material begins to expand, and heated material cools. This very general description covers scenarios that range from the Big Bang, to thermonuclear explosions in stars, to magnetohydrodynamic explosions on the sun and to most of the chemical explosions on the Earth.

The intent of this issue on explosions is to expose the reader to some of the many different aspects of explosion phenomena known today. The articles here address a variety of theoretical, computational and experimental studies of explosions, thereby demonstrating the range of methods employed in investigations. In addition to presentations of background knowledge, underlying theoretical formulations and their mathematical exposition, each article contains previously unpublished research that opens up new questions and issues for future study. An initial summary, given next, of a few basic concepts, which in subsequent articles are assumed to be known by the reader, may facilitate understanding of the material that is to follow.

2. Fundamentals

The basis of our present understanding began with the experimental observations of Berthelot & Vieille [1] and Mallard & LeChatelier [2], and the theoretical explanations of Chapman [3] and Jouguet [4], more than a century ago. Notable advances were made by Zel'dovich [5], von Neumann [6] and Döring [7], among many others, who identified elements of the structure (the ZND structure) of detonations, which are the stronger of the two classical types of explosions. The names of these nine scientists have been thoroughly associated with the fundamental concepts that they developed. These concepts identify two distinct steady-flow regimes, to which time-dependent explosions may evolve, or between which time-dependent explosive transitions may occur.

It is instructive to consider the pressure–volume (p–v) diagram of a fluid as shown in figure 1. The pressure p_0 and specific volume v_0 of the initial mixture are indicated as a point in this diagram. For steady, planar, one-dimensional flow, principles of conservation of mass, momentum and energy can be used to find the locus of possible final states of the fluid after the heat release has occurred in an explosion. That locus, called the *Hugoniot curve*, as illustrated in the figure, consists of two disconnected parts, an upper branch and a lower branch. The two branches must be separated for exothermic processes because application of steady mass and momentum conservation alone requires that a straight line

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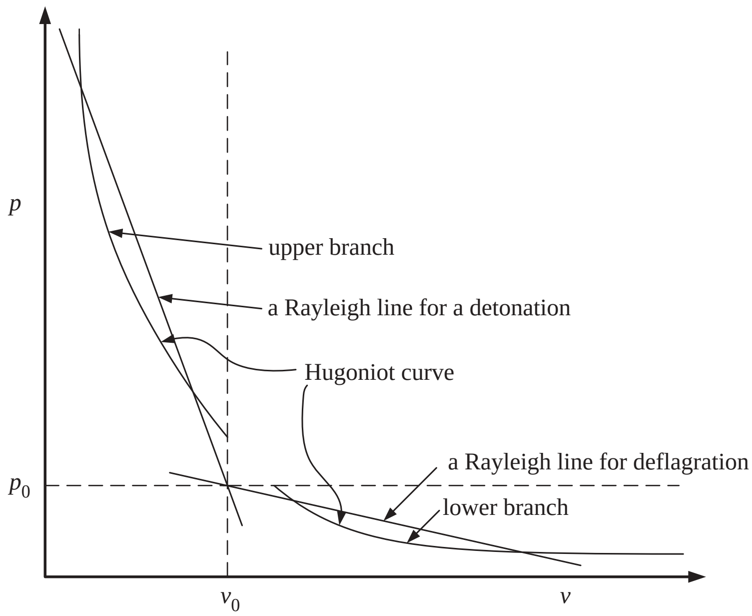

Figure 1. Traditional pressure–volume (p–v) diagram showing the Hugoniot curve with possible states of deflagrations and detonations.

connecting the initial and final states in this diagram, called the *Rayleigh line* (known in gas dynamics as a trajectory for constant-area compressible flow with heat addition), cannot have a positive slope. When the final state lies along the lower branch of the Hugoniot curve, the process is called a *deflagration*, and when it lies along the upper branch, it is a *detonation*.

Thus, there are two very different and distinct types of one-dimensional, steady reaction waves propagating through homogeneous reactive material, consistent with conservation conditions. The figure illustrates that detonations exhibit large pressure increases and small volume decreases, while deflagrations have large volume increases and small pressure decreases. Propagation velocities of such fronts are proportional to the square root of the negative of the slope of the Rayleigh line, two representative examples of which are indicated on the figure. Propagation velocities of detonations are thus seen to exceed those of deflagrations; detonations are found to be supersonic and deflagrations subsonic. The figure also shows that there is a minimum velocity for detonations and a maximum velocity for deflagrations, limiting conditions that correspond to tangency of the Rayleigh line and the Hugoniot curve, and the associated final conditions are called the (upper and lower) *Chapman–Jouguet* (*CJ*) *points* of the curve. Further analysis demonstrates that final fluid velocities are sonic at the CJ points.

Except for CJ conditions, when there is any intersection at all between a given Rayleigh line and the Hugoniot curve, there are two, as can be seen in the figure. Therefore, there are two different types of each process. From the slopes, it is seen that both types of deflagrations travel slower than CJ, and both types of detonations faster. The first intersection is called weak and the

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second strong. Final fluid velocities are supersonic for strong deflagrations and for weak detonations, while they are subsonic in the other two cases. Although strong deflagrations have been postulated for certain galactic winds, all known deflagrations on the Earth are weak, approaching CJ only for highly turbulent, energetic flames. On the other hand, most detonations are CJ, although both weak and strong detonations occur. Strong detonations often arise for periods of time in transitions from deflagrations to detonations (DDTs). Laboratory studies of chemical kinetics in shock tubes, when exothermic overall, in principle also are strong detonations for the entire shock-tube test time. On the other hand, condensation 'shocks' in wind tunnels are weak detonations.

Explosions, however, are dynamic processes that often are neither the classical deflagrations nor the classical detonations described by steady-state flows in homogeneous backgrounds with perfectly unobtrusive geometries. As an example, consider the preceding conclusion that detonations are supersonic and deflagrations subsonic; this will be seen in a later article to not always be true for porous media. Although pressure changes associated with deflagrations are smaller than those associated with detonations, the expansion and heating that occur in deflagrations cause pressure build-up, especially in confined spaces. This can be quite damaging and thereby causes the processes to be classified as explosions, even though detonations do not develop. In many instances, these pressure waves and their associated heating produce DDT. The most damaging explosions, however, are generally detonations because they have the highest pressures. Pressures even higher than those in CJ detonations can occur in transient processes, such as shock–shock interactions and strong detonations, which precede the completion of DDT. Depending on the specific configuration and both the reactivity and the energetics of the combustible mixtures, periods may occur in which there is supersonic front propagation slower than CJ, and such slow (sometimes called 'weak') detonations are types of explosions that may not transform fully to CJ and that cannot be classical steadily propagating fronts. Nevertheless, they may be very damaging and therefore need to be understood. There thus exist many non-classical types of explosions requiring further study.

3. Topics in this Theme Issue

The first article in this issue presents an examination of one of the largest recent accidental chemical explosions. The explosion at Buncefield, UK, in 2005 is unique in that it is unusual to have such a thorough investigation of a large-scale, accidental, statistically improbable event. Questions raised by the forensics committee included the following. What caused the fuel spillage? How did it ignite? Do we know enough to understand the dynamics of the turbulent flame development and propagation? What was the role of the obstacles in the path of the explosion front? And finally, did a detonation develop at any stage? This first article, by Bradley *et al.* [8], summarizes the work of the technical investigation committee, presents the current state of the analysis of this event, puts it in the context of other historic large-scale accidental explosions and then describes where future research is required. This needed research, such as the research reported in the subsequent articles in this issue, goes well beyond the idealizations identified earlier.

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The ZND detonation structure envisions steady, planar flow with heat release initiated by the temperature rise across a strong planar shock wave (as in many shock-tube experiments). Evidence that this picture is much too simplified for most real-world explosions can be at least traced to the observations of spinning detonations by Campbell & Woodhead [9], and clear recognition of the prevalent existence of multi-dimensional structures was provided by Denisov & Troshin [10]. We now know that the ZND structure is generally unstable, evolving into cellular detonation structures that range from regular diamond patterns to very complex dynamic interactions of shock waves, reaction regions and shear layers behind leading shock fronts. In the second article, Kessler *et al.* [11] use multi-dimensional numerical simulations to study these phenomena. By extending the computations to detonation propagation normal to a gradient of stoichiometry, they identify upstream (behind the detonation front) reaction regions into which reactants diffuse from opposite sides. This region is bounded by rich and lean reaction regions, and the result is a triple-flame detonation wave. This type of gradient of fuel concentration could develop in the more complex spatial and temporal fuel distributions that occur in explosion-prone situations, such as in tunnels in coal mines or during industrial fuel leakages.

Complementing this computational work are the analytical studies in the third article; Clavin & Williams [12] present a unified formulation that covers a range of detonation topics, including initiation, propagation, quenching, pulsation and cellular structure. Asymptotic analyses are discussed here for the limit of strongly temperature-sensitive rates of heat release and for the Newtonian limit in which the difference between constant-pressure and constant-volume heat capacities vanishes (assumed by Isaac Newton and found to be surprisingly accurate for high-temperature real gases in hypersonics). Planar detonations are shown to be unstable to shear-wave disturbances, even when the heat-release rate is insensitive to temperature, with a weakly nonlinear analysis indicating that this bifurcation leads to distinct diamond patterns. This article also clarifies conflicting literature concerning the stability of shock waves in general non-ideal fluids, deriving for the first time the boundary between decaying and non-radiating, non-decaying stable shock discontinuities.

The next two articles are theoretical and experimental investigations, respectively, of explosions in porous media. The first, by Brailovsky *et al.* [13], summarizes implications of a simplified mathematical model based on the concept of hydraulic resistance. Introduction of the hydraulic-resistance approximation reduces the order of the differential equations that describe the detonation and deflagration processes, thereby facilitating their solution and making it easier to understand their predictions. For these reasons, it is important to determine experimentally the extent to which the model can correspond to reality, and a new favourable comparison is identified (called Shchelkin's effect there). The experimental observations and measurements reported by Ciccarelli [14], in the second of these articles, expose experimental similarities and differences between explosion propagation in porous media and in chambers filled with obstacles. These results are quite revealing; they show, in particular, structures of explosions in the low-velocity slow-detonation regime, where the propagation velocities of the fronts are between c_s and the CJ detonation velocity. It is made clear here that acquisition of detailed, local data on explosions in porous media is

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a challenging experimental task. These studies are important, especially to the extent that porous-media results can be applied to industrial-accident situations with obstacles in the flow.

The authors of the next article, Chiquete & Tumin [15], follow in the path of investigators who have performed mathematical stability calculations of planar detonations. Here, they specifically consider, for the first time, influences of slightly porous walls in circular tubes, and they compare their results with those for an impenetrable wall. The analysis and associated numerical results provide a clear example of effective methods for tackling problems of this kind.

The next two articles, again the first somewhat more theoretical and the second somewhat more experimental, address the development of explosions in various types of chambers and for various combustible mixtures. Bradley [16] first explains a well-developed, coherent viewpoint of the explosion processes in spark-ignition, internal-combustion engines. This study of explosions, which are at the smallest scale considered in this issue, indicates how and when engine knock may occur. Ideas are extended to explosion development in ducts, including a summary of results for turbulent deflagration velocities. By contrast, Thomas [17] summarizes results of extensive experimental studies of DDT, both in gaseous and in solid explosives. In addition to addressing a number of different processes, such as detonation development in gradients of fuel concentration and the transmission and diffraction of detonation waves at junctions, the interactions of different scales in explosion phenomena are described. A major concern of Thomas has been to produce experimental results on very hard problems that are amenable to further study and analysis by numerical simulations. An example of this, described in the article, is the 'strange wave' phenomena, involving the coupling of a shock, a flame and a boundary layer.

The last two articles strike out in quite different directions. First, Starikovskiy *et al.* [18] describe the physics and chemistry of plasma-assisted ignition in combustion processes, and then they show how this can be used to promote DDT for use in engines that employ detonations for propulsive purposes, either continuously, as in rotating-detonation engines, or periodically, as in pulsed-detonation engines. Plasma-assisted combustion is an extensive topic in itself, one that requires consideration of ionized states of atoms and molecules. Although knowledge of the complex kinetics of such ionized states has been developed for specific applications, such as atmospheric and ionospheric chemical reactions or solar coronal thermonuclear reactions, they are not generally known for the usual hydrocarbon molecules involved in combustion problems. The authors of this penultimate article describe what is known, and we can thus infer how much we will need to learn to properly use plasmas to enhance combustion.

Finally, Wheeler [19] addresses the many types of astrophysical explosions currently under discussion in astrophysics, bringing us up to date on some of the latest work and theory. These explosions include magnetohydrodynamic and thermonuclear energy sources, mentioned previously, and gravitational collapse is also considered. It is noteworthy how atomic, nuclear and plasma physics interact with turbulence and transport of particles, photons and neutrinos as critical ingredients in these problems, which involve extraordinarily wide ranges of relevant scales. Explosions of white-dwarf start lead to type Ia supernova (SNIa), which have become the 'standard candles' of our Universe. Wheeler discusses how measuring SNIa spectra and red shifts leads to the most consistent determination

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of the rate of expansion and size of the Universe. Understanding why SNIa are so uniform involves understanding the evolution of turbulent flames and detonations in the thermonuclear environment in the star, which certainly is a challenging topic in explosions.

4. Other future research directions

An important question not addressed in the following articles concerns explosion limits. It is commonly accepted that there are reactive mixtures which are too dilute, too fuel lean or too fuel rich to explode under any circumstances. Moreover, the literature contains extensive tabulations of flammability limits for various combustibles, specifying, for example, upper and lower deflagration limits, such that deflagrations cannot persist in mixtures richer than the upper limit or leaner than the lower limit. There are also explosion-limit diagrams, in which explosions are known to occur spontaneously in mixtures lying between these limits; these spontaneous explosion limits are narrower than deflagration limits and are of less interest in the present context. In addition to deflagration limits, there are detonation limits, although less data are available for detonations. Despite a common belief that limits of detonability are narrower than deflagration limits, fundamentally this need not be true. The chemical kinetics of detonations differs from deflagrations in that they require initiation steps in which chain carriers are formed, while the chain carriers are already present in deflagrations. To delineate mixtures in which the most severe types of explosions may occur, it is of interest to determine limits of detonation.

It is well known that limits of detonation of combustible mixtures in chambers depend on the dimensions of the chamber. A detonation propagating past a stationary wall develops a boundary layer on the wall behind the leading shock, and the influence of this boundary layer on the flow can tend to weaken the detonation. For a detonation in a long circular tube of diameter d, the propagation velocity decreases with decreasing values of d, and at a critical diameter, the propagation ceases. The value of this limiting diameter depends on the composition of the mixture. Figure 2 is a graph of experimental results for the value of $1/d$ at this critical diameter for methane–air mixtures initially at room temperature and normal atmospheric pressure [20–22]. It has been standard procedure to extrapolate such plots to $1/d = 0$ to define detonability limits of combustible mixtures in the open. It may be seen from this figure that, prior to 2011, this extrapolation would have led to the conclusion that methane–air mixtures with less than 6 per cent or more than 14 per cent methane on a volume basis would lie outside the limits of detonation. However, the recent data seen in the wings clearly demonstrate that this conclusion would be false. Tabulated detonability limits for methane are in error. Further research to determine ultimate limits of detonation is warranted. As it becomes increasingly difficult to generate explosions in such near-limit mixtures, it is important to also study what is required for their initiation.

Another significant area of investigation is the control of explosions. Depending on the particular situation, there is interest in generating explosions, preventing them, or quenching them once they develop. There are many different ideas about explosion control. One article in this issue discusses the use of plasmas for control.

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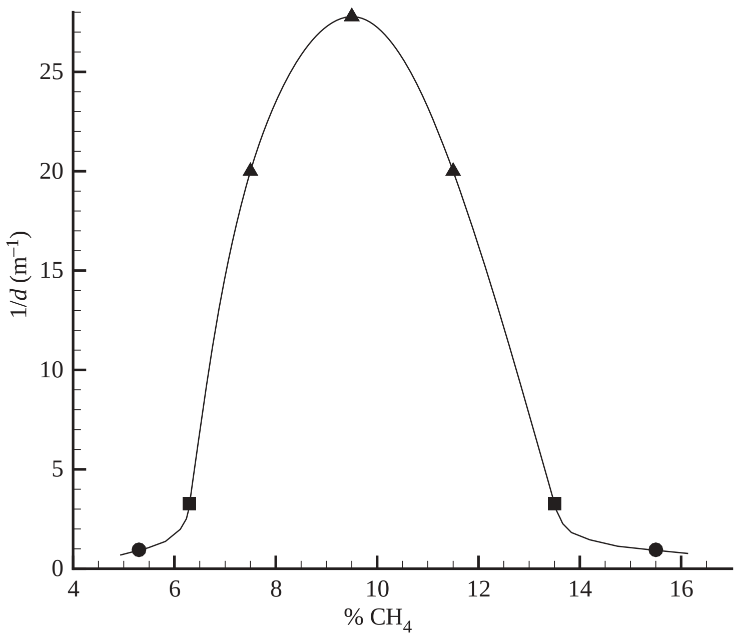

Figure 2. Measured lean and rich detonation limits for methane in air as a function of the per cent of methane by volume. Limits are shown for four values of $1/d$, the inverse of the diameter of the test device. Names and symbols refer to earlier studies (squares, Kogarko [20]; triangles, Matsui [21]; circles, Gamezo *et al.* [22]).

Relief valves and blow-out caps are common explosion-control devices. There have been studies of detonation arrestors, for example, employing narrow channels, porous materials, dust dispersions, water sprays, water-filled passages, etc. There have been methods for extinguishing explosions that attempt to disperse inert rock dust or placing buckets of water to be overturned during an explosion. But the task is confusing and difficult. Methods that appear to damp explosions under some conditions enhance them under other conditions. We would like to be able to control transients, to change the explosion state, so that we can ignite, enhance or quench at will, turn detonations into deflagrations or taylor the process of DDT. Much more understanding is necessary to achieve these objectives.

Finally, more research is needed on the role of turbulence in explosions. A half-century ago, when the ZND detonation structure was widely accepted as universal, fine-scale shadowgraph observations surprisingly suggested that detonations were turbulent. Improvements in resolution soon showed that this turbulence, in reality, was the now-familiar regular cellular diamond pattern. Today, with greatly improved experimental techniques, especially for detonations having highly irregular, somewhat chaotic cell structures, reacting shear layers behind leading shocks are often described as turbulent. The true nature of this kind of turbulence, however, remains to be determined. As high-speed deflagrations interact with shock waves and boundary layers, they are subject to shock-related and shear-flow instabilities that may generate turbulence of character different from that which is commonly understood. More thought is thus warranted about turbulence in all types of explosions.

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There is now a great deal of knowledge about turbulence in fluids, which has been employed to construct diagrams for turbulent combustion, with different types of combustion processes reasoned to occur in different parts of the diagrams. One selection of coordinates for such a diagram is a turbulence Reynolds number and a turbulence Damköhler number, the ratio of a turbulence time scale to a chemical time scale [23]. Turbulent combustion is considered to occur in a distributed manner at low Damköhler numbers and in sheets at high Damköhler numbers, for example. Questions arise, however, as to whether such a classification is sufficient for explosions.

In a recent computational study showing DDT in unconfined systems [24], compressibility effects suggest that a Mach number should be considered as a coordinate for classifying regimes of turbulent combustion. This possibility remains to be explored. Turbulent combustion computations for SNIa employ classical turbulence concepts, but in that application, the associated Lewis number, the ratio of the heat diffusivity to the reactant diffusivity, is very large, of the order of 1000 or more. Even laminar deflagrations, however, are known to be unstable to pulsating instabilities at large Lewis numbers, approaching a pulsating type of chaos, a turbulence quite different from that known for fluids, for Lewis numbers greater than about 10, thereby calling into question the basis of the standard candle. Consideration therefore perhaps should be given to including the Lewis number as a coordinate for diagrams of turbulent combustion. Thus, much remains to be learned about turbulence in explosions.

5. Concluding comment

The breadth of topics covered by the word 'explosions' is enormous, ranging, for example, from solid explosives used in mining and demolition to nuclear explosions for interplanetary travel, from gamma-ray bursts to air-bag inflators. In all of these, the basic underlying physical principles share much in common, but the specific materials, applications and scenarios differ wildly. In this brief introduction, we have first tried to summarize the most fundamental explosion concepts that underpin all of the articles that follow. We have then attempted to emphasize at least one important aspect from each of the articles and, at the same time, to point out the relationships among the different topics. Each article also indicates directions for future research, which we have supplemented with a short (and certainly incomplete) description of current problems that are not covered in depth in the articles. We hope that this brief introduction and the articles that now follow will provide useful perspectives on explosions.

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