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Understanding explosions – From catastrophic accidents to creation of the universe

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Abstract

This paper focuses on two extremes of explosions: the general class of Type Ia supernova (SNIa), which are surprisingly uniform thermonuclear explosions of white dwarf stars, and a specific gasoline vapor-cloud explosion that occurred at the Buncefield fuel depot in 2005. In both cases, recurring questions are whether an initial spark or small, local ignition could result in a detonation, and if so, how could this happen? The broader question is: What is the origin of the deflagration-to-detonation transition (DDT) in confined, partially confined, and unconfined systems? The importance of DDT to SNIa is based on the use of these objects as cosmological "standard candles" that are used for measuring distances and curvature in the universe. The importance of DDT to Buncefield is related to design and operational safety of industrial plants and fuel storage facilities. Combinations of observations, specific laboratory experiments, and selected numerical simulations have given us information and some understanding of the DDT process and its likelihood. Numerical simulation both of large- and small-scale phenomena in these reactive flows were important ingredients in the studies. The invention and discovery of numerical algorithms, including (but not limited to) monotone methods, implicit large-eddy simulation, and adaptive mesh refinement, enabled these simulations certainly as much as the increase in computer speed and memory. Unresolved issues that arose in these studies include the nonequilibrium, non-Kolmogorov properties of the turbulence and turbulent fluctuations in these flows, how these prepare the system for transitions, and how to represent the chemical reactions and energy release in the high temperatures and pressures that are near and might signal a transition.
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Keywords: Chemical explosions; Type Ia supernova; Deflagration-to-detonation transition; Numerical simulations of high-speed compressible flow

Preface

This is *not* a review paper. Instead, it is a selective compilation of information and results from studies of the extremes of combustion that range from cosmology to micropropulsion. This paper presents a story of progress in two specific areas of combustion – accidental explosions and astrophysics – and attempts to show how knowledge from one field informs and advances another. The paper also slips in several issues from a long list of problems that confront the future use of numerical simulation of reacting flows.

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The form of this paper was partially inspired by frustrating efforts to create a recent edited volume for the *Philosophical Transactions of the Royal Society*, Special Issue on *The Physics, Chemistry and Dynamics of Explosions* [1]. The contents of that volume of collected papers could only skim the surface by presenting a relatively small slice through a universe of information on chemical and astrophysical explosions. It described some of what we have done to understand these incredible, magnificent, malicious, and creative events.

Several reviewers commented that the paper was "rather qualitative," or to paraphrase, "too many words and not enough equations." On reflection, I think that might be true,but it is misleading. The format is the result of an effort to bring the reader up to speed in many areas of research as quickly as possible. In fact, an enormous amount of experimental, theoretical, and computational work, enough for a long review article or several books, is too often summarized in a sentence or two. Unless that was done, I saw no way to make some of the points needed to proceed with the arguments. In an effort to satisfy the reviewers, I added a small, more quantitative section describing one of the most important concepts, the ignition of gradients of reactivity.

I gratefully acknowledge the family, friends, and colleagues with whom I have worked closely over the years to build up a base of knowledge and capability. If you do not read anything else, please read the acknowledgments and savor every name there.

1. Introduction

At every scale, explosions are defining features of our universe, as they "destroy order and create new states and directions" [2]. In combustion, an explosion can signal a transition from a deflagration to a detonation or the formation of a strong shock front by a turbulent flame. Explosions are a fundamental part of astrophysics [3,4]. For example, an explosion signals the transformation of a star from a white dwarf to a supernova, which enables the creation of the heavier elements, neutron stars, or black holes. The transition in the early universe from quarks to baryons has been studied as a detonation wave (see [5,4] has more references). We might argue that the Big Bang itself is an explosion that marks the beginning of our universe. Besides their creative aspects, explosions have a downside. Large-scale accidental industrial explosions are rare events with disastrous consequences for human life and property. Recent occurrences, such as Buncefield [6] Jaipur [7], Sago Mine [8], or Toulouse [9], made international headlines. Many other smaller-scale, less publicized events have also cost dearly. Sometimes we can decipher the chain of events that led to the explosion. Sometimes we can identify a way to change the background in some way to decrease the likelihood of a recurrence. Sometimes, any control is beyond us, and we can only observe with awe or shock.

Whereas the common use of the term *explosion* can be ambiguous, we can give it a more technical definition [2]. An explosion ...

" ... refers to any type of scenario in which energy is injected into a system faster than it can be smoothly [acoustically] 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 Alfvén 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, strong pressure waves (shock waves) develop and spread outward, traveling 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, to most of the chemical explosions on earth."

This description of an explosion resulted from discussions that came about as we tried to find a definition inclusive enough to cover the broad range of situations we were considering. In the process, we argued whether or not the Big Bang, which creates space-time as the universe expands, was really an explosion that fits into any normal definition of the word. This paper, however, focuses on chemical explosions, such as those that occur in fuel depots or coal mines, and by analogy on thermonuclear explosions, such as those that occur in supernovae.

1.1. Steady-state physics – review and terminology

Common ideas of chemical explosions identify two distinct, steady-flow combustion regimes, subsonic flames and supersonic detonations. Many types of transitional states occur as a system undergoes transitions between these steady states. Figure 1, an example of the "$p-v$ diagram," encapsulates much of our current understanding and is a starting point in studies of combustion. An initial, unexploded mixture is