THE STRUCTURE OF PROPAGATING DETONATIONS: LESSONS FROM NUMERICAL SIMULATIONS

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Since the early 1900's, the general understanding of the structure of detonations has developed from the simplest theories that account for global features to a considerably more complex and dynamic picture. Instead of the idealized one-dimensional picture of a planar detonation with instantaneous heat release at the shock front, (the Chapman-Jouguet theory), we now know that the front of a self-sustained detonation propagating in an energetic gas is neither uniform nor planar. The structure is complex and multidimensional, involving interactions between incident shocks, Mach stems, transverse waves, and boundaries of the regions through which the detonation is moving (see, for example, [1–3]). Initially, information about the structure of detonations was obtained experimentally from smoke-foil measurements, and then later from other methods such as schlieren and open shutter photography. These measurements were accompanied by extensive theoretical analysis. This work provided the underpinnings of what we now know, and selected aspects are covered by other presentations in this minisymposium.

More recently, it has been possible to add numerical simulations to the arsenal of tools used to study detonation structure. There are two major contributing physical processes in gas-phase detonations – local energy release and compressible fluid dynamics – that need to be coupled to represent a detonation. Because of this apparent simplicity of the contributing physical processes, there have been extensive efforts in recent years to simulate detonation structure. However, the apparent simplicity disappears and the subject becomes infinitely more complex and dramatic when multidimensional fluid interactions, multispecies, multistep chemical kinetics, or nonideal equations of state are considered.

In the early 1970's, computing the properties of a one-dimensional unsteady detonation with a reasonable chemical model was a chore. Now we can do this for two-dimensional simulations and, to some extent, for three-dimensional detonations. This new capability has arisen from both the development of robust numerical algorithms and an enormous increase in our computational resources. The numerical algorithms are robust monotone methods that can solve the time-dependent compressible reactive Euler and Navier-Stokes equations and reliably capture shocks. Accessible computational resources, the computer speed and memory, have increased to the point where what had to be done on a 1970's supercomputer can now be done on a small desktop workstation [4].

In this presentation, information derived primarily from multidimensional numerical calculations is compiled and used to explain the structure of detonations, including the occurrence and importance of transverse shock waves, cellular structure, creation of unburned detonation pockets behind the wave front, and irregularity of detonation cells. It is shown that detonation cells are likely to occur in many types of detonations, ranging from frequently encountered chemical systems to thermonuclear supernovae. Finally, information on detonation decay, reignition, and propagation is combined to describe the behavior of a transmitted detonation wave.

Cellular Structure of Propagating Detonations

The unsteady structure of a detonation results from of the continuous motion of a system of colliding and interacting shocks. Since the first numerical simulations [5–7], many simulations have confirmed that the region around shock triple points (the intersection of the transverse shocks, Mach stems and the incident shocks) trace out the patterns we call detonation cells. This verification was the first step in producing a database that yields much more detailed information about detonation structure.

In fact, such simulations have shown and, to some extent explained, features that are often hard to decipher from experiments. For example, a standard gas mixture for studying detonation cells is low-pressure H_2-O_2. Computations of detonation propagation in such mixtures first showed the transverse wave structure [5] and then showed that these evolve into detonation cells [6]. Subsequent computations showed details of the Mach structure at the detonation front as the cell evolves [8]. The system evolves from a single Mach reflection, to a double Mach reflection, and then to even more complex shock structures. Even more recent computations that used a detailed chemical reaction model have shown even more complexity in the cellular patterns [9], and seen in the background graphic of the 17th ICDERS poster.

Unreacted Detonation Pockets

One initially unexpected but potentially important feature found in the experiments and simulations is the formation of unreacted pockets of material behind the detonation front [6,7]. Experiments first showed such pockets, but their implications were unexplored until they were seen in numerical simulations.

The formation of the pockets can be traced directly to the curvature of the transverse shock waves. When two transverse waves collide or one hits a wall, the interaction can cut off a portion of unreacted, cold material from the chemical induction zone. If the material in the pockets burns slowly enough, the process effectively draws energy out of the detonation and can provide a mechanism for detonation extinction. If the pockets burn rapidly, they can generate pressure pulses that perturb the front, perhaps leading to new transverse waves. These findings are curious because they show how an initially homogeneous material can develop an extremely inhomogeneous structure as shocks move through it. The existence of unburned pockets provides a multidimensional fluid-dynamic mechanism by which a detonation can die in a situation where, in one dimension, it might be expected to propagate.

The initial discussions of unreacted pockets were for mixtures of hydrogen and oxygen in narrow channels with decaying detonation waves. Since then, the existence of pockets has been shown to be much more common and to occur in many materials, in wide channels, and for nondecaying detonations. Recent work has shown that stronger triple points are associated with larger pockets and more irregular cell structures, and the state of the pockets varies as the effective activation energy of the material increases [10,11]. For self-sustained detonations, the pockets burn quickly enough for the effects of the energy release to be felt by the detonation front, and the delayed burning supports the detonation. When the burning occurs behind the front by a length of approximately one or two detonation cells, the pockets extract energy from the detonation front. In the discussions below, we refer to the pockets as they affect properties of astrophysical supernovae and reignition in layered detonations.

Complex and Irregular Cell Structures

For most energetic gases, the picture described above is still too simple. The cellular structure of most propagating detonations is usually much more complex: sometimes there are smaller cellular substructures within a detonation cell, and sometimes the detonation cells are very irregular. These effects can be traced to the complexities in different chemical reaction mechanisms and to the differences in thermophysical properties of the material.

For example, detonation cells created in some materials contain substructures that themselves resemble either a full or partial cells. One explanation for this kind of structure and substructure is that there are sequential chemical reactions, in which there are multiple induction and energy-release stages. This has been observed recently in experiments in gaseous nitromethane [12], and it is the case for the computed cellular structure resulting from thermonuclear detonations [13].

Recent parametric studies [10] have correlated irregular structure with strong triple points and large unreacted pockets, both of which occurred at high activation energies. The cellular structures computed for the conditions in Type Ia supernova all appear somewhat regular, but quite complex due to the complex reaction mechanism [13]. This is, in effect, a high-activation energy system. Unreacted pockets are observed

for all of these structures.

To date, these various results for quite different reaction models seem to have contradictory results. The unreacted pockets seem universal, and may be present for most systems, either regular or irregular. Unifying all of these results into a set of concepts consistent with each other and experiments is a topic for future research.

Universality of Cellular Structure

Type Ia supernovae are the brightest known stellar objects and most frequent type of supernovae observed. They are believed to be explosions of white dwarf stars that have accreted enough mass to be unstable and explode. A single explosion releases approximately 10^{51} ergs of energy into the interstellar medium, and these explosions are the major source of all iron-group elements formed in the universe. Because of the constancy of the energy release and the uniformity of the their spectra, Type Ia's are used as "standard candles" to estimate the age, size, and curvature of the universe by comparing their intrinsic luminosity to their apparent brightness.

Thermonuclear burning in supernovae involves many reactions of nuclei from hydrogen to zinc. The main reaction in the explosion is $^{12}C + {}^{12}C$, which produces oxygen and releases $\simeq 50\%$ of the available nuclear energy. The remaining energy is released by a subsequent complicated reaction chain that produces nuclei from carbon to nickel with protons, neutrons and α-particles. An important question is where and when the explosion proceeds as a turbulent flame or a detonation.

The chemical and physical parameters that are required for a numerical simulation of a supernova blast are better known that those in any but the most idealized terrestrial combustion systems. The difficulty is that the disparities in scales are even larger than in terrestrial problems. The radius of an unexploded white dwarf, is $\simeq 2 \times 10^8$ cm, and expands during the burning phase to $\simeq 10^9$ cm. Depending on the density, the thickness of a laminar nuclear flame in a carbon-oxygen white dwarf is $\simeq 10^{-3} - 10$ cm, and the thickness of the carbon detonation front is about one hundred times larger, $\simeq 10^{-1} - 10^3$ cm.

Recent numerical simulations [13] of the multidimensional structure of a detonation propagating in this thermonuclear material has been shown that there are three somewhat distinct stages in the thermonuclear reaction mechanism: the first stage is carbon burning, the second is oxygen burning, and the third is silicon burning. Because of the disparity in the timescales of the three reaction processes, the cellular structure appears to have extremely disparate scales, ranging millimeters to kilometers in scale. An important effect of the cellular structure is tied to the creation of unreacted pockets on the largest, silicon scale. In these cases, the existence of such large pockets could mean that a detonation is extinguished sooner that would be predicted from standard one-dimensional estimates.

Layered Detonations and Transmission

We conclude the presentation by describing simulations [14] that examined the diffraction, decay, and reignition that occurs when a detonation propagates into a region of increased cross-sectional area [15]. Consider a detonation propagating in a tube containing a shoichiometric H_2-O_2 mixture at 1 atm, 300 K. At some point, the bottom wall of the tube ends abruptly, and the detonation expands laterally (is transmitted) into either the same mixture or one of another dilution or stoichiometry. Because of the expansion, the reaction front decouples from the leading shock and forms a decaying blast wave ("bubble") followed by a reaction front (a turbulent flame). Then, depending on the initial conditions, the shock and reaction front either continue to decouple or detonation reignites. It might reignite "spontaneously" before the leading shock reaches the bottom wall, or it might reignite as a result of the leading shock reflecting from the wall and forming a hot region. In some cases, the detonation may appear to "gallop" as it reignites, only to decay again, reignite, and so forth.

Simulations of this process show the importance of the unsteady dynamics of the transverse waves and the changing and adapting cellular structure to predicting the transmission process.

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