Detonation: A Look Behind the Front

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The nature of detonation fronts in gases has been investigated experimentally and theoretically for over 100 years and yet, key questions remain unanswered. Foremost among these are the issues of front instability and the role of transverse shock waves in the reaction process. Detonation front instability creates fluctuating conditions within the reaction zone, most importantly: temperature fluctuations created by variations in the main shock front speed and the presence of counter-propagating systems of transverse shock waves. In addition to these temperature fluctuations, the three-dimensional nature of the shock configuration at the front, associated triple-lines, and unstable contact surfaces create regions of high shear in the flow that will promote mixing between regions with very different degrees of reaction progress. Since chemical reaction rates are a strong function of both temperature and radical species, the fluctuations may have a profound effect on the rate at which reaction occurs and how rapidly chemical energy is converted to the thermal energy. In particular, models such as the classical Zel'dovich-von Neumann-Doring (ZND) reaction zone (Fickett and Davis 1979) based on average properties and quasi-steady variations behind a mildly perturbed shock front may have to be completely abandoned in some cases. This is obviously an extreme position and one-dimensional ideas will continue to be useful conceptual tools. At the same time, these classical ideas may be limiting our imagination and it is useful to explore what we know about detonation fronts today with an open mind toward constructing new paradigms.

The issue of fluctuations in detonation fronts is very analogous to that faced in turbulent combustion twenty years ago: Is it adequate to model a flame as a highly distorted and strained laminar front - or do the fluctuations completely disrupt the front and require a description in terms of "distributed" combustion? Further, what is the proper way to couple the usual statistical description of small and intermediate-scale motion in turbulent flows with a deterministic flame structure that converts reactants to products in a spatially organized fashion? If we replace the word "flame" with "detonation reaction zone", we see that we are confronted with exactly these same issues today in detonation research. Resolving these issues appears to be central to progress in all aspects of predicting detonation behavior, since fluctuations within detonation fronts are a universal aspect of all gaseous detonations. In doing so, it may be helpful to draw on the substantial repertoire of concepts (Peters 2000, Poinsot and Veynante 2001) developed by the low-speed turbulent combustion community.

Background

There has been a very substantial amount of work on detonation carried out by previous researchers, including the founders and participants in this Colloquium. These studies have been very important in defining the fundamental issues in detonation front structure. We may roughly divide these studies into two categories. First, there have been detailed optical observations of the near-front region using schlieren, shadowgraph, and interferometric measurements of the density profiles. Second, measurements of initiation, propagation, and failure of detonations in various geometric configurations have been carried out for a variety of combinations of fuels, oxidizers, and diluting compounds. For example, observations have been made of minimum initiation energy, limiting tube diameter for propagation, critical tube diameter for diffraction, and failure distance in channels with porous walls. These quantities are sometimes referred to as "dynamic" properties to distinguish them from the properties such as the Chapman-Jouguet (CJ) velocities and pressure, which can be computed from thermodynamic considerations alone.

The key result from the detailed studies of the front is the notion of cellular structure, the name being motivated by the characteristic patterns created on soot foils placed in detonation tubes. The importance of the cellular structure is that it indicates the existence of a quasi-periodic spatial and temporal oscillation in the leading shock strength and a system of weak shock waves propagating transversely to the front. From elementary chemical kinetic considerations, these oscillations in shock strength must be accompanied by large oscillations in reaction rate that result in spatial variations in reaction rate behind the front. Although early experimental measurements unambiguously showed the transverse wave systems and lead shock fluctuations, the intense fluctuations in density behind the front and the integrating nature of the optical methods made it impossible or extremely difficult to directly observe the fluctuations in reaction rate.

The key result from dynamic property measurements is that the intrinsic length and time scales associated with the detonation front structure provide natural dimensions to scale the critical quantities such as initiation energy. However, it is very significant that the observed macroscopic length scales such as critical tube diameter are at least two orders of magnitude larger than the nominal reaction zone length. This indicates that the processes of detonation initiation and failure involve subtle effects that spread the influence of unsteadiness and wave front curvature out over a large portion of the wave front.

Numerous experimental observations of the cellular structure have been made in laboratories throughout the world (Shepherd and Kaneshige 1997) by using the soot foil technique. Measurements of a characteristic "cell size'' have been made and found to be very useful in developing empirical correlations for detonation initiation and transmission limits. These correlations and similar correlations with ideal (ZND) reaction zone length are essentially dimensional analysis and provide no new insight into actual physical and chemical mechanisms of detonation initiation or failure. In addition, it is extremely difficult to quantify detonation cell size measurements except in the case of very regular cellular structure. While cell size methods will continue to be an important tool for engineering analyses of detonation behavior, it is clear that the progress of future research will require a detailed understanding of the processes within the reaction zone.

There are a bewildering variety of results available on detonation front structure, the relationship to chemical kinetics, and the dependence of the dynamic parameters on the specific chemical system. I have selected a few key issues that stand out when surveying the past work and comment on each.

1. *Universality of cellular structure.* Cellular structure appears to be present in all self-sustaining gaseous detonations. However, this may not be the same cellular structure for all mixtures. The degree of organization or regularity of the cellular structure is a strong function of the chemical composition. Highly organized or regular structures occur only in mixtures that are highly diluted (greater than 60%) with rare gases such as argon. Hydrocarbon fuel-oxygen and, to a greater extent, fuel-air mixture cellular structures are much more disorganized than those of rare-gas diluted mixtures and the most disorganized cellular structure is observed in mixtures that contain inhibitors (bromine compounds) or are diluted by high heat capacity. The current conceptual model (Fickett and Davis 1979) of detonation front structure as a quasi-periodic configuration of transverse waves propagating near the sonic velocity is heavily biased by the extensive experimental studies done on argon-diluted mixtures in narrow channels. At the time of those studies, this configuration gave the best possibility for understanding the details of the front in isolation. However, now that we are able to resolve the details of the front for a wider range of mixtures, we see that detonation front structure may not be universal and that concepts applicable to very regular structures may not be as useful for irregular structures.

2. *Role of chemical kinetics in cellular structure.* Much of the research on this issue has focused on trying to find simple, chemically-based length scales and figures of merit that correlate with the measurements of cell size. The most important observation is that the ZND model can be used with detailed chemical kinetics to compute a reaction zone length that serves as a reference length in correlating cell width. Beyond this simple but very useful result, the relationship between cellular structure and chemical kinetics is unclear. The ratio of cell width to reaction zone length can vary systematically from 10 to 100 with variations in the chemical composition. More significantly, chemical composition is a key factor in determining the extent of disorganization of the cellular structure. The role of activation energy in linear stability theory and phenomenological models was recognized early on, and experimentally, there is a clear correlation with increasing activation energy resulting in increasingly disorganized structures. Cellular structure is, of course, a very nonlinear phenomenon and cannot be analyzed just on the basis of the linear stability theory. However, it seems natural to refer to mixtures with very regular cellular structure as “weakly unstable” and mixtures with irregular cellular structure as “strongly or highly unstable”. This is an issue that will remain unresolved until we develop the capability to do direct simulation with detailed reaction mechanisms and corresponding instability analyses in order to determine how the spectrum of linear and nonlinear instability modes depends on the chemical system.

3. *Dynamic Behavior and Cellular Regularity.* Mixtures with highly irregular cellular structure behave differently in dynamic situations than do mixtures with highly regular cellular structure. For example, in hydrocarbon fuel-air mixtures with irregular structure, the critical tube diameter for successful diffraction from a confined to an unconfined situation is about 10-15 times the detonation cell width. For mixtures highly diluted with argon and regular structure, the critical tube diameter can be as much as 40 times the cell width. Similar systematic variations are observed for other dynamic properties when comparing mixtures with irregular vs. regular

> cellular structure. A particularly clear example of this is given by Radulescu and Lee (2002) for the case of detonation failure when propagating through a channel with porous sections. Mixtures with regular cellular structure fail slowly, propagating a distance of up to 100 cell widths after entering the porous section. Mixtures with a highly irregular structure fail rapidly, propagating only a distance of about 4 cell widths after entering the porous section. On the basis of this behavior and related observations for other situations, they have proposed that the combustion process is distinctly different in mixtures with an irregular cellular structure as compared to those with a regular cellular structure. In particular, they propose that transverse wave collisions are very significant and a type of turbulent combustion may be taking place in mixtures with irregular cellular structure as compared to a laminar process in mixtures with regular cellular structure.

To summarize, there is a very substantial amount known about detonation front structure in the regime of regular cellular structure that occurs in mixtures highly diluted with argon. Much less is known regarding the highly irregular regime and there are indications that the combustion process may be quite different than the observed laminar process that proceeds according to the classical concept of shock-induced branching chain-thermal explosions being convected behind the front. The key question underlying all of the issues raised by the previous research is:

“What is the nature of the combustion process within the detonation front and how does this depend on the chemical composition of the reactants?”

The goal of our work is to answer this question by developing concepts and constructing explicit models that can be used for engineering estimates of detonation dynamic parameters for a wide range of chemical systems. An essential first step is the experimental characterization of the spatial and temporal distribution of chemical reaction within the front.

Recent Experimental Studies

Experimental studies of the structure of gaseous detonation fronts started after the Second World War and were made possible by the development of high-speed photographic methods, miniature piezo-electric pressure transducers, and the high-speed oscilloscope. Essentially the same techniques are in use today with light sources provided by lasers instead of sparks and digital computers and cameras are used instead of cathode ray tubes and film. Soot foil measurements are essentially unchanged in technique since 1875, requiring only waste fuel oil and sheet metal. However, a significant advancement in technology has been the widespread availability of tunable coherent light sources, particularly dye lasers with very precise wavelength control. Coupled with this is the development of sensitive electronic imaging systems that enable recording images in short (10-100 ns) time intervals. It is these two developments that enable the visualization and measurement of specific chemical species within the reaction zone. In our laboratory, we have used the traditional measurement techniques alongside laser technology to image planar slices of the detonation front simultaneously with the integrated density field.

From an experimental point of view, we would like to accomplish two things. First, to characterize the geometry of the reaction front and quantify the spatial and temporal distribution of reaction rate within the front. Second, to investigate how the “equilibrium structure” that is set up in a propagating detonation responds to disturbances created by external events such as diffraction through an opening or passage through a tube or channel lined with porous material. At Caltech, we are currently in the first phase of this process and have been visualizing (Pintgen 2000, Shepherd et al. 2002, Pintgen et al. 2002, Pintgen et al. 2003, Austin 2003) the chemical species behind the leading shock front for several chemical systems.

Observations are presented for a range of mixture compositions exhibiting different degrees of cellular regularity in Figs. 1-6. The mixtures are arranged in order of increasing effective activation energy. The properties of the mixtures are specified in Table 1. These images were obtained in two different facilities, a 150 X 150 mm square test section at the end of a 7.3-m long, 280-mm diameter detonation tube (GDT) and an 18 X 150 mm rectangular channel, 4.2 m in length (NC). Both facilities have special initiator systems that minimize startup transients and produce self-sustaining detonations with near-CJ velocities in the test section region.

For each mixture class, one laser schlieren image showing the density field is presented and several OH planar laser induced fluorescence (PLIF) images are shown to illustrate slices through the OH concentration field behind the leading shock front. The leading shock wave is usually clearly visible on the schlieren images and depending on the regularity of the structure, transverse shock waves can also be identified. For the more irregular mixtures, the leading shock front has a diffuse appearance due to the three-dimensional nature of the front and the integrating character of the schlieren method. This is particularly true in the larger test section but is also the case in the narrow channel for more irregular mixtures. A distinct OH front is also observed in the PLIF images. Although the OH concentration increases continuously behind the shock front, the appearance of a sharp front is due to the exponential growth of the concentration by the branching chain mechanism and the sensitivity characteristics of the intensified camera. Physically, this OH front corresponds to a contour of constant OH concentration if all other factors are the same. Fluctuations in the location of the OH front relative to the nominal shock location reflect the sensitivity of reaction rates to temperature variations, primarily created by fluctuations in the strength of the leading shock.

H_2-O_2-Ar Mixtures (Fig. 1) - These mixtures have very regular cellular structures, and an organized system of transverse waves is visible in the schlieren image. The normalized effective activation energy E_a/RT_{vN} is approximately 5 for this case. In the PLIF images, the OH front is smooth and a periodic variation in the front location is observed, resulting in a very characteristic feature that we term a "keystone". Reasonable agreement between postulated and observed "keystones" is obtained using simple gas dynamic concepts and quasi-steady reaction zone models that assume laminar flow and the traditional concept of periodic cellular structure. We find that only modest increases in the reaction rate occur across the transverse waves and that the transverse waves do not play an essential role in the combustion process. Shear layers emanating from the triple-lines are visible in some schlieren images but not in the OH PLIF images.

H_2-O_2-N_2 Mixtures (Fig. 2) - These mixtures have less regular cellular patterns but the OH fronts still appear smooth and have the characteristic keystone features with irregular boundaries marked by Kelvin–Helmholtz instability and vortex rollup on the shear layers, especially for larger amounts of diluent. The normalized effective activation energy E_a/RT_{vN} is approximately 6 for this case. Regions of low OH concentration appear to be lagging behind the main front. It is not known at

this time, if these are indeed isolated (surrounded by reacted material) pockets in the flow field or if they are an artifact of visualizing a three dimensional front with two-dimensional slices.

H_2-N_2O-O_2-N_2 Mixtures (Fig. 3) – These mixtures mark the appearance of small scale fluctuations on the OH front and a fine structure on the leading shock front. The normalized effective activation energy E_a/RT_{vN} is approximately 7 for this case. This agrees with the previously observed appearance of a "cellular substructure" on the detonation front. Some keystones and vortex structures similar to Fig. 2 are visible in the PLIF images.

H_2-N_2O-N_2 Mixtures (Fig. 4) The OH fronts show fluctuations with a wide range of length scales and the shock front has a diffuse fine structure. The normalized effective activation energy E_a/RT_{vN} is approximately 8-9 for this case. The range of OH front fluctuation length scales is even larger than in Fig. 3 and isolated holes or pockets of low OH concentration appear to be embedded within higher OH concentration regions. Some remnants of the keystone features are visible as are some individual vortices at the boundary between high and low OH concentration.

C_2H_4-O_2-N_2 Mixtures (Fig. 5) In this figure and the following one, the cellular structure is very disorganized and a large range of fluctuation length scales are visible. Substantial regions of low OH concentration appear near the end of the cell cycle, suggesting that the reaction rates are very low due to the effects of unsteadiness and the low value of the leading shock velocity at these times. With some imagination, keystone structures can be visualized but the boundaries are quite distorted. Regular trains of vortex structures or even isolated vortices are not observed. The normalized effective activation energy E_a/RT_{vN} is approximately11-12 for this case.

C_3H_8-O_2-N_2 Mixtures (Fig. 6) This case is very similar to the one shown in Fig. 5. The normalized effective activation energy E_a/RT_{vN} is approximately13 for this case. Bright spots, regions of high OH concentration, are observed close to the regions where transverse waves interact. High-speed camera records indicate explosive events taking place at these locations.

The evolution shown in Figs. 1-6 of the shock and OH fronts with increasing effective activation energy is quite striking. The most obvious effect is the appearance of fine scale disturbances on the OH and shock fronts for E_a/RT_{vN} greater than 7. The presence of these disturbances imply that there are localized, rapid fluctuations in shock strength occurring at characteristic lengths that are 10 to 100 times smaller than the largest scale – the so-called dominant cell width. These fluctuations are superimposed on the large-scale oscillations of the shock front, which are manifested as the keystones visible in Figs. 1-3 and larger regions of low OH concentration observed in Figs. 4-6. For example, in Fig. 5d, the very smallest fluctuation scales resolvable by the imaging system are less than 1 mm while the large-scale motion is on the order of 100 mm.

Even in mixtures with regular cellular structure (Fig. 1), fluctuations will have a significant effect on the average reaction rate since the excursions in temperature are quite large. As shown in Fig. 7a, the lead shock oscillates in speed from about $0.9U_{CJ}$ to $1.3U_{CJ}$ for a weakly unstable detonation front (high argon dilution). The probability distribution function for shock speed (Fig. 7b) is significantly skewed to speeds lower than CJ but also has a long tail at high velocity. These shock speed excursions correspond to post-shock temperature swings from a low of 1600 K to a high of 3000 K as compared with a post-shock state of 1950 K for a shock traveling at the average speed of

U_{CJ}. Instead of examining the effect on reaction rate, it is more conventional in detonation studies to consider the induction time associated with a given shock velocity. Computations of the induction time based on the constant-volume approximation are shown for two representative mixtures in Fig. 8. Mixture A corresponds to the case shown in Fig. 7 and the induction time is predicted to vary between the extremes of 9 and 0.5 μs with the CJ value being at 3.5 μs. Mixture B corresponds to cases similar to Figs. 5 and 6 with a more extreme variation in induction time than Mixture A due to the higher activation energy.

For mixtures with high activation energies and highly irregular cellular structures, the shock velocity history and probability distribution functions are unknown and will have to be determined through either experimental measurement or direct simulation. There are indications from simulations and experiments that an even larger range of shock speed variations may be present (0.6 to 1.6 times the CJ speed) than in the case of regular structure. The combination of large fluctuations in shock velocity and a high activation energy creates at least two very significant complications.

First, enormous excursions in induction time will occur for high values of E_a/RT_{vN}. For example, Mixture B in Fig. 8 has $E_a/RT_{vN} = 10$. For the same range of shock speed variations as shown in Fig.7, the induction time is predicted to vary between 29 and 0.1 μs with a CJ value of 3.5 μs. This variation by a factor of 300 in the induction time is one obvious explanation for the origin of the large range of sizes of fluctuations observed in highly irregular mixtures. For the larger range of shock speed variations that may be possible in high activation energy mixtures, the induction time may vary by up to a factor of 10^3.

Second, fluctuation intensities larger than a critical level can completely extinguish the chemical reaction process. The existence of these critical fluctuation levels can be inferred from the study of Eckett et al. (2000) who found that unsteadiness in the reaction zone behind a decaying shock wave could compete with the chemical energy release and cause quenching of the reaction process. This will create regions of shocked and partially reacted gas that may subsequently explode due to cooperative effects like a spontaneous flame (Swacer) mechanism or else undergo rapid reaction following the collision of transverse waves in such a region. This suggests that temporal oscillations in the shock strength may play a role in detonation fronts analogous to strain in low-speed flames. Rapid fluctuations in shock strength may be responsible for disrupting the continuity of the reaction zone and producing the highly corrugated OH fronts observed in Figs. 4-6.

Implications for Engineering Models of Detonation Fronts

As scientists, we appreciate the basic research goal of *direct numerical simulation* to compute all relevant physical phenomena with resolution sufficient to accurately represent all spatial and temporal variations. Essential insights into the fluid mechanics and combustion processes are obtained in this fashion and we expect that direct simulation will play an important role in resolving the nature of the combustion process in highly fluctuating detonation fronts. The development of adaptive mesh methods and parallel computation have enabled the direct simulation at the level of the Euler equations (no diffusive processes) for weakly unstable reaction zones and regular cellular structure with detailed reaction mechanisms for simple mixtures like $2H_2$-O_2-7Ar in two (Oran et al. 1998, Eckett 2001, Deiterding 2003) and three (Deiterding 2003) dimensions.

As engineers, we appreciate that the brute force attack of direct simulation is not a viable approach for industrial problems. In typical explosion hazard engineering computations, the characteristic length scales are meters as compared to the mm size fluctuations in the OH front or the 1-10 μm spatial resolution required for computation of species evolution between the shock and OH front. Direct simulation even has severe limitations for very idealized situations if we try to treat hydrocarbon combustion or include diffusive processes that may be relevant to mixtures with highly irregular cellular structure. The difficulty is both the spatial resolution required to resolve diffusive scales and the computational resources required to carry out direct simulations with a large (greater than 50-100) number of species. Although there has been a great deal of progress in developing reduced reaction mechanisms for many hydrocarbon fuels, these techniques are far from mature and validation of these approaches will ultimately require direct simulation with a full mechanism. Finally, extensive experience with low-speed turbulence simulation indicates that direct methods are limited to regions of extremely small spatial extent and modest Reynolds numbers when the diffusive processes are fully resolved. Even with ongoing advances in software and hardware, it simply will not be possible to carry out fully resolved simulations of detonation initiation and propagation for industrial problems that we will need to handle in the next decade or two.

These considerations about resolution and direct simulation suggest the need for models of the detonation front that can represent the processes that we know exist but, for practical reasons, are unable to resolve. In the context of turbulence in nonreacting flows, these are known as subgrid-scale models and are used to represent the effects of turbulent motion and dissipation at length scales smaller than the finest resolution used in the computation. These models are particularly important to simulating high Reynolds number flows since the length scales at which viscous dissipation occurs is approximately $Re^{-3/4}$ times the largest length scale. For detonation simulation, the subgrid-scale model must also include the processes of chemical reaction within the unresolved regions. The large range of spatial scales and disorganized appearance of the small-scale structure visible in Figs. 4-6 suggest that a statistical approach may be appropriate.

One obvious way to go about modeling the effect of fluctuations is by using a presumed shock speed pdf like Fig. 7. Fluctuations in shock speed translate directly into temperature fluctuations that cause fluctuations in reaction rates, which determine the species concentration profiles. However, a strictly stochastic model of a fluctuating shock front is unlikely to be sufficient. Even in highly irregular mixtures, spatial and temporal correlations will exist due to the acoustic waves and fluid motion within the reaction zone. Cooperative phenomena like spontaneous flames and transverse wave collisions are also known to play a role in high activation energy mixtures. Even if we ignore these correlations and cooperative effects, the closure of a statistical model for the reaction process in a fluctuating detonation front requires considering how the fluctuations influence the combined chain-branching thermal explosion that takes place behind the shock front. This is quite a different problem than the usual issue of premixed or diffusion flames for which specialized methods like G-equation methods or flamelets have been developed. It is likely that a completely new methodology will have to be developed to handle the present situation.

In addition to considering the effects of fluctuations on the reaction rate, the role of diffusive transport may need to be reevaluated. The conventional wisdom is that diffusive processes are too slow to contribute to the combustion process in detonation fronts. However, this may need to be reconsidered given the very small spatial scales observed on the OH fronts for high activation energy mixtures and the mixing potential of the high Reynolds number shear layers that exist behind the triple point lines.

Conclusions

Previous research on detonation front structure indicates that there are significant differences between detonations in mixtures with high effective activation energy and low effective activation energy. These differences point to the possibility of qualitative differences in the combustion process itself and we are led to pose the following question: "What is the nature of the combustion process within the detonation front and how does this depend on the chemical composition of the reactants?" In the case of low activation energy mixtures, experimental and computational studies give a reasonably complete picture of a fluctuating laminar reaction zone with a combined chain-thermal explosion process that is controlled by the oscillations in the lead shock velocity. In the case of the high activation energy mixtures, visualization experiments show a highly disturbed shock front followed by an OH front with substantial spatial disruptions. Considerations about reaction rate dependence on shock strength and fluctuation rate suggest that fluctuations within the reaction zones in these mixtures may qualitatively alter the nature of the combustion process as compared to laminar process observed in the low activation energy mixtures. For engineering modeling of industrial problems and even for many laboratory-scale experiments, subgrid-scale models of unresolved processes within the detonation front will be required.

Acknowledgement

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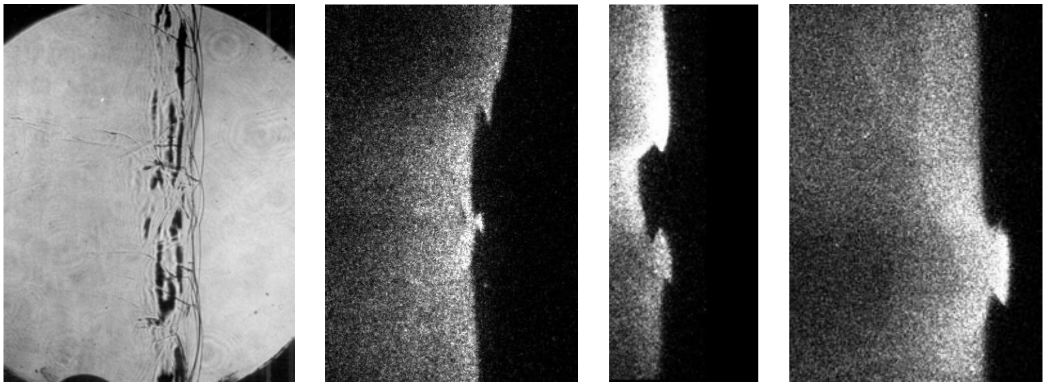
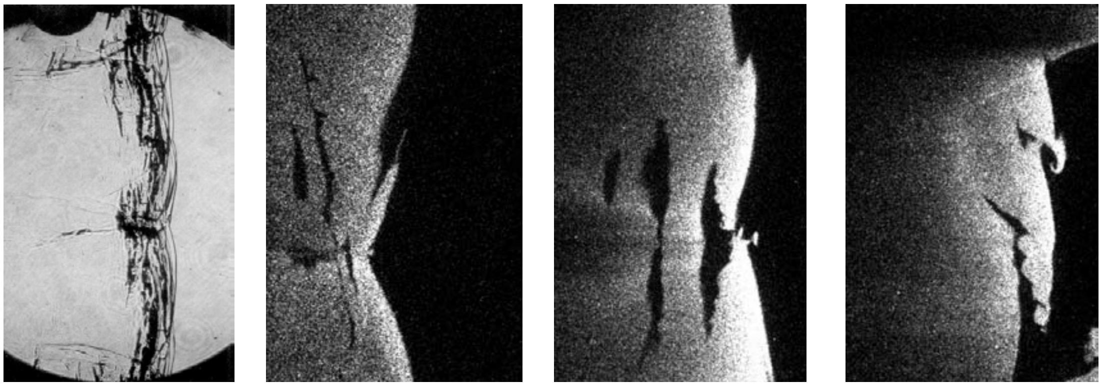


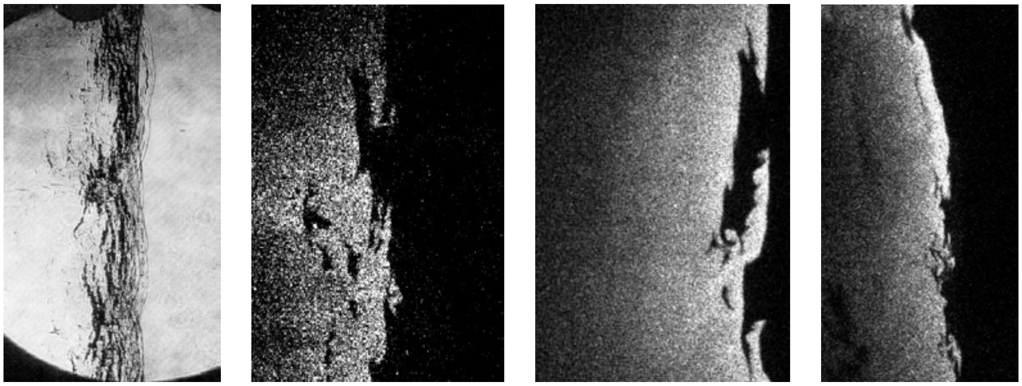
a) b) c) d)

Figure 1. Schlieren and PLIF images of detonation fronts in H_2-O_2-Ar mixtures.



a) b) c) d)

Figure 2. Schlieren and PLIF images of detonation fronts in H_2-O_2-N_2 mixtures.



a) b) c) d)

Figure 3. Schlieren and PLIF images of detonation fronts in H_2-N_2O-O_2-N_2 mixtures.

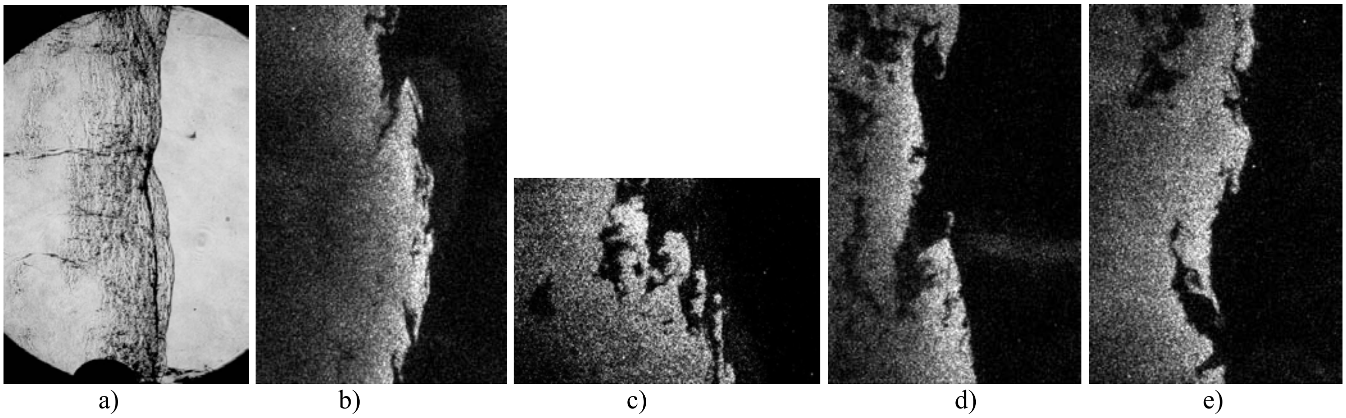

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Figure 4. Schlieren and PLIF images of detonation fronts in H_2-N_2O-N_2 mixtures.

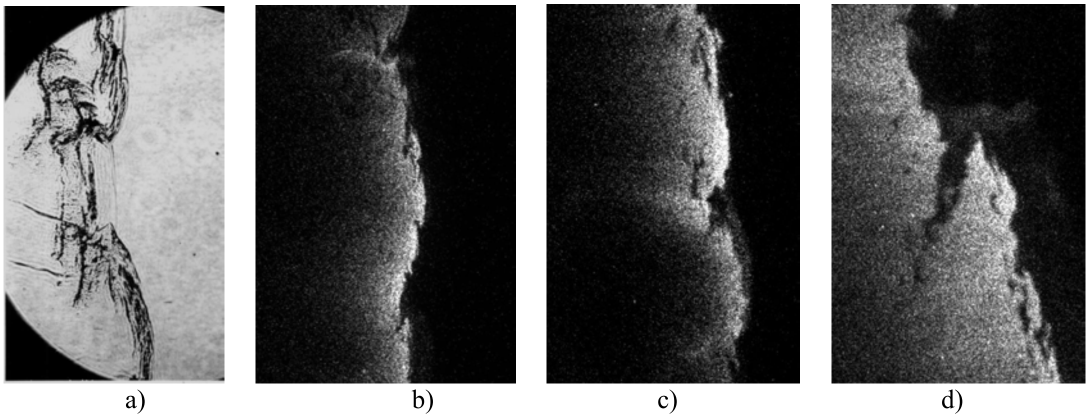
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Figure 5. Schlieren and PLIF images of detonation fronts in C_2H_4-O_2-N_2 mixtures.

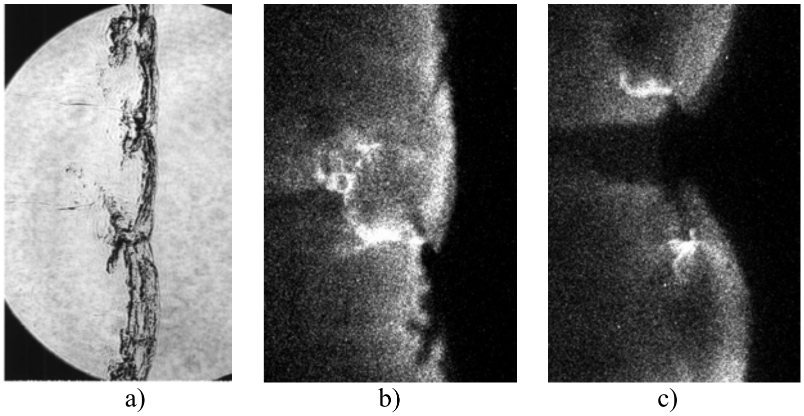
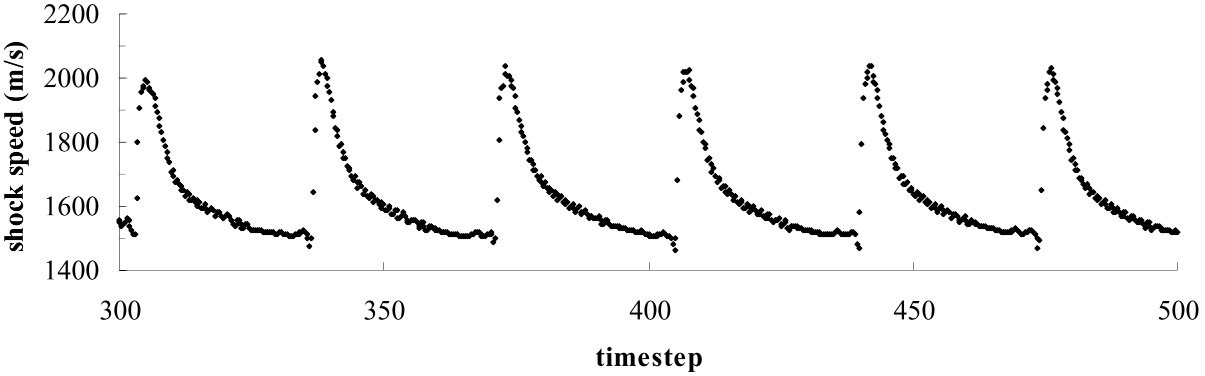

a) b) c)

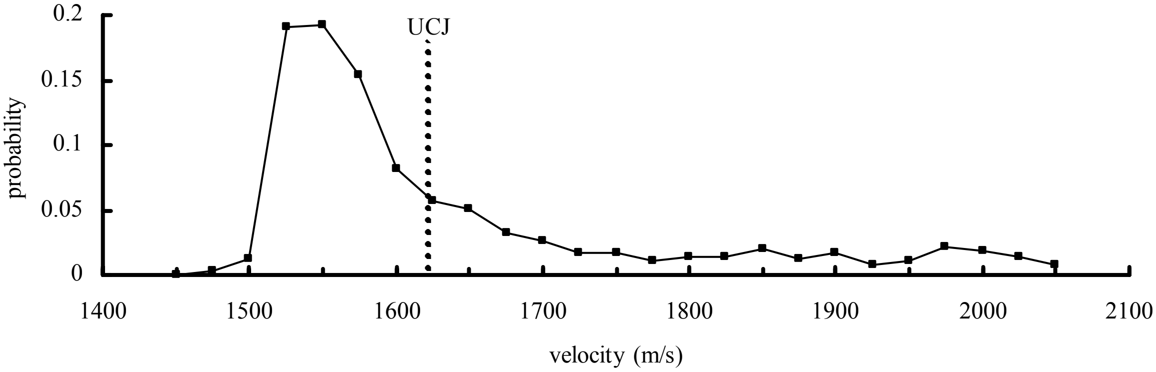
Figure 6. Schlieren and PLIF images of detonation fronts in C_3H_8-O_2-N_2 mixtures.

Table 1. Index to Figs. 1-6, schlieren images of the detonation front (first in each row) and Planar Laser Induced Fluorescence Images of the OH radical distribution behind the detonation front in mixtures with various regularity. The detonation is travelling from left to right in all images. Two facilities were used to obtain these images: The Gaseous Detonation Tube (GDT), with a 150mm square test section, and the high aspect ratio Narrow Channel facility (NC), with a cross section of 18x150mm. The facility used, shot number, mixture composition in moll fractions, initial pressure and height for each image shown is given below. All mixtures are stoichiometric and the initial temperature for all shots was 294K.

Fig	Shot No.	Mixture	PO (pa)	Image Height (mm)
1a	GDT1676	8.6H2-4.3O2-87AR	20	150
1b	GDT1581	10H2-5O2-85AR	20	58
1c	GDT1651	10H2-5O2-85AR	20	69
1d	GDT1596	8.6H2-4.3O2-87AR	20	29
2a	GDT1680	22H2-11O2-67N2	17.5	150
2b	GDT1678	22H2-11O2-67N2	17.5	30
2c	GDT1681	22H2-11O2-67N2	17.5	30
2d	GDT1604	22H2-9O2-73N2	20	45
3a	GDT1664	24H2-3O2-18N2O-55N2	13.5	150
3b	GDT1671	24H2-6O2-12N2O-58N2	11.3	51
3c	GDT1686	24H2-6O2-12N2O-58N2	30.4	30
3d	GDT1684	24H2-3O2-18N2O-54N2	13.5	30
4a	GDT1608	20H2-20N2O-60N2,	20	150
4b	GDT1685	25H2-25N2O-50N2	30.4	30
4c	GDT1687	20H2-20N2O-60N2	20	29
4d	GDT1608	20H2-20N2O-60N2	20	45
4e	GDT1609	20H2-20N2O-60N2	20	45
5a	NC173	C2H4-3O2-10.5N2	20	150
5b	NC69	C2H4-3O2-9N2	20	60
5c	NC87	C2H4-3O2-9N2	20	60
5d	NC175	C2H4-3O2-9N2	20	30
6a	NC188	C3H8-5O2-9N2	20	150
6b	NC188	C3H8-5O2-9N2	20	30
6c	NC205	C3H8-5O2-9N2	20	60



(a)



(b)

Figure 7. (a) Time series (Accept 2000) of lead shock velocity computed for 2H2+O2+7Ar detonation, two-dimensional regular cellular structure; (b) probability distribution function for shock velocity time series shown in part (a).

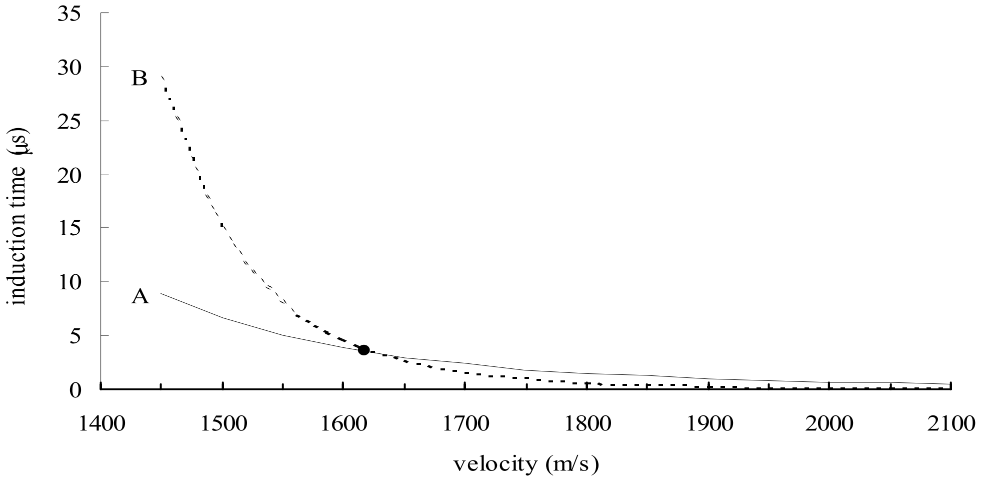


Figure 8. Induction time as a function of shock velocity for mixtures with two different effective activation energies and a common CJ induction time. Mixture A corresponds to 2H2+O2+7Ar with $E_{a.}/RT_{vN}$ is approximately 5, which is a mixture with very regular cellular structure. Mixture B corresponds to typical hydrocarbon fuel-air mixtures with E_a/RT_{vN} is approximately 10, a mixture with a highly irregular cellular structure.