

Liquid-Fueled Detonations in Tubes

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Motivated by the current interest in pulse detonation engines, a brief review of previous work on liquid-fueled detonations in tubes is presented. Although the characteristics of detonations in high-vapor-pressure liquid fuels are analogous to those of gaseous detonations, the behavior of detonations in low-vapor-pressure liquid fuels is quite different. The multidimensional structure and the cell sizes of such mixtures have not yet been established. Theoretical, computational, and experimental studies have shown that if the droplets are fine enough (less than about 10 μm), detonations propagating at about the equivalent gas-phase Chapman–Jouguet detonation velocity can be attained in a variety of fuel–oxygen systems. With larger droplet sizes, a deficit in the propagation velocity compared to the gas-phase velocity is observed. Various explanations for this deficit are presented. The droplet size required for detonations in fuel–air mixtures is smaller than that in fuel–oxygen mixtures. Heating the initial mixture helps both by easing the detonation initiation process and by aiding in the detonation propagation by introducing some prevaporization and reducing the droplet size. The need for additional research on multiphase detonations to aid in the further development of liquid-fueled detonation engines is also emphasized.

Introduction

ALTHOUGH detonations involving particulate matter have been known in the context of mine and grain elevator explosions for a long time, systematic studies involving liquid-fueled detonations appear to have begun only in the 1950s.¹ Since detonation or detonation-like phenomena were observed in liquid aerosols in an oxidizing gaseous atmosphere,² propulsion applications have often been cited as a motivation for the study of liquid-fueled detonations. The motivations have included basic concerns about propulsion devices utilizing standing or traveling detonations,^{3,4} development of liquid-fueled rocket engines,^{5,6} understanding of nonlinear combustion instability,^{7–9} and more recently renewed interest in pulse detonation engines (PDEs).^{10–25} Most of the PDE-related work to date has focused on gaseous mixtures.^{26,27} Both these reviews discuss multiphase detonations because for many practical applications that are volume and weight-limited, the PDE will require the use of a liquid fuel. With liquid fuels, additional issues such as atomization, droplet breakup, partial vaporization, and incomplete fuel–air mixture (to name a few) must also be considered. Parameters such as droplet size and temporal and spatial distribution of droplets will play a major role. Our understanding of the structure, stability, detonability, and initiation of liquid-fueled detonations are all more primitive than for detonations in gaseous fuel–oxidizer mixtures. The objective of this report is to briefly review past and more recent work that may have an impact on further development of liquid-fueled detonation engines.

There has also been a vast amount of work pertaining to multiphase detonations involving solid particulates in a gaseous medium (for example, Refs. 28–39). A large amount of reference material can be found that documents the detonation characteristics under such conditions and how various fuels, geometries, and initiation energies affect the detonation properties (see for example Refs. 28, 33, 37, 38). Although of general interest to multiphase

detonations, many of these studies are not directly applicable to liquid-fueled detonation engines. Hence, they have not been discussed further in this paper. Interested readers can find an extensive discussion of detonation waves in dust media in review articles by Lee³³ and Zhang.³⁸ There are also many studies involving thin liquid fuel films inside tubes. Early works by Sichel et al.,⁴⁰ as well as later studies by Borisov and Maikov,⁴¹ aid in characterizing such detonations and their propagation. Although not the main focus of this paper, such studies are of some relevance to detonation-based propulsion systems, because some of the injected fuel is likely to be deposited on the tube walls. Some other studies on hazards posed by fuel–air clouds^{42–44} also provide basic information relevant to the development of liquid-fueled detonation engines.

In this paper, the early systematic studies of spray detonations that took place in the 1960s are discussed first. This not only serves to acknowledge the pioneering studies but also provides an outline for the rest of this paper. These early studies brought out the observation of a velocity deficit (compared to the Chapman–Jouguet (C-J) detonation velocity) and the need to consider processes beyond heterogeneous droplet burning behind a shock wave to account for the detonation structure. Then various conceptual models of the detonation structure are presented, followed by discussion of the effects of droplet size and tube diameter. Observations of detonations in unconfined fuel clouds are used to motivate a discussion of detonability and initiation requirements. This naturally leads to a discussion of cellular structure of detonations. On this as well as other topics, the reader is cautioned to interpret the observations in the context of the vapor pressure of the fuels under the conditions investigated: low-vapor-pressure fuels behaving quite differently from high-vapor-pressure fuels. Before the concluding remarks, a brief report is also made on developments in numerical simulation of liquid-fueled detonations.

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Early Systematic Studies of Spray Detonations (1960s)

The basic importance of addressing “questions concerning the existence, structure, and stability of detonations in sprays” in developing operational propulsive devices based on detonations was raised by Williams^{3,4} as early as 1961. The focus of his one-dimensional theoretical analysis was on a nonvolatile fuel spray in a gaseous oxidizer. Considering a situation with “maximum possible deviation” from a purely gaseous detonation, Williams^{3,4} hypothesized a spray detonation wave to consist of a shock wave followed by a heterogeneous deflagration where the fuel burned to completion in the surface layer of the droplet. The analysis showed the existence of detonation solutions to the one-dimensional spray conservation equations but raised some issues about the structure and stability of such detonations. For fuel sprays of radius 30 μm (diameter 60 μm) in air, the size of the burning region was on the order of 1 m, indicating that non-one-dimensional interactions including heat losses to the walls that were neglected in the analysis would become important, casting doubt on the stability of such spray detonations. A smaller reaction-zone length and stronger coupling with the shock front were to be expected if shattering of the droplets or significantly smaller droplets were considered.

The development of reliable liquid rocket engines motivated Webber⁵ and Cramer⁶ to conduct what are generally acknowledged to have been the first systematic experiments on spray detonation. Their shock tube studies showed the onset of detonation-like phenomenon and even at that time, Cramer⁶ suggested that mechanical shattering of the droplets must have taken place to “produce enough of a less than 10-micron droplet mist to provide sufficient fuel vapor” to drive the detonation front. He also noted that a high equivalence ratio was needed to sustain the detonation-like wave.

A series of papers published in the mid to late 1960s reporting on studies of Dabora et al.,⁷ Ragland et al.,⁸ and Dabora et al.⁹ were “motivated by the current belief that liquid rocket motor instability can result in a detonation or *detonation like* phenomenon.” Diethylcyclohexane (DECH— $\text{C}_{10}\text{H}_{20}$)—gaseous oxygen was used in all experiments because of its purity, low volatility, and properties comparable to those jet fuel RP-1. Dabora et al.⁷ conducted three types of experiments: 1) detonation in a polydisperse spray, 2) detonation in a thin film on the tube walls, and 3) detonation in a monodisperse spray. In the first type of sprays, with an estimated mean droplet diameter of 200 μm , propagation velocities well below the theoretical C-J velocities were observed. They thought that only a fraction of the fuel might be entering the initial reaction zone and hence increased the equivalence ratio but did not see a significant change in the propagation velocities. In the case of the thin films, steep-fronted waves were observed with even lower velocities. In the case of monodisperse sprays with mean droplet diameters of 940 μm , velocity deficits of about 30% were observed. They also extended the analysis of Williams³ to account for specific heat variations across the shock/detonation front, but the results were very similar.

Ragland et al.⁸ focused on a single dilute stream of 2600- μm droplets dispersed in gaseous oxygen and used streak and space-resolved photography to view details of the droplet breakup behind a shock wave. They concluded that the time required for complete disintegration of a 2600- μm droplet was about 500 μs and including combustion in the wake of the disintegrating droplet, the time required increased to about 670 μs . Heat transfer to the walls could be significant during that time and they estimated that 20% of the heat of reaction could be lost. They suggested that this could account for the 32% detonation velocity deficit that was observed compared to the equivalent gaseous mixture.

Dabora et al.⁹ summarized the DECH experiments, focusing on the droplet-size (290, 940, and 2600- μm) effects. The spray detonations were initiated using a stoichiometric hydrogen–oxygen detonation wave. They appear to have been the first to state that “the developmental time of a spray detonation decreases with decreasing drop diameter.” That is, the smaller the droplet size, the faster the detonation developed into a steady state. The steady velocity was lower than the C-J velocity, with a deficit of 2–10% for the smaller droplet sizes and 30–35% for the 2600- μm droplets, as shown in

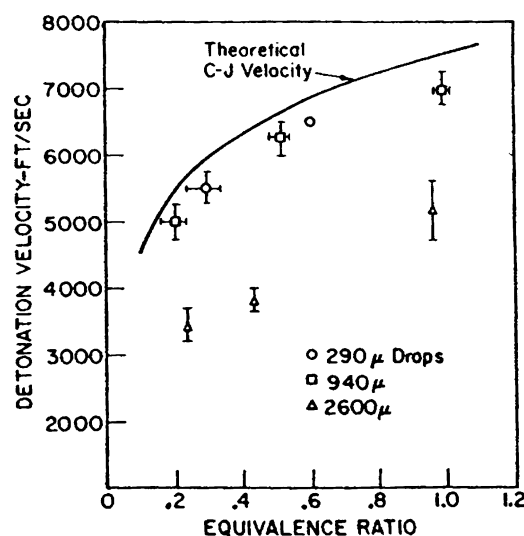


Fig. 1 Comparison of the measured detonation velocity with the ideal gas-phase C-J velocities (from Ref. 9).

Fig. 1. They also invoked frictional losses to the walls in conjunction with a reaction zone length controlled by the breakup of droplets to arrive at a relationship that directly related observed velocity deficits to droplet sizes.

Several key observations can be made from these pioneering studies. First, the structure of a liquid-fueled detonation is more complex than that of a shock wave followed by the heterogeneous burning of droplets. Processes such as droplet breakup and the presence of fuel vapor appeared to be essential to explain the observation of detonations. When detonations occurred, propagation at sub-C-J velocities was noted. This velocity deficit (compared to the C-J detonation velocity) was correlated to the droplet size. Long reaction zones and consequent losses to the walls were thought to be the reason for the observed velocity deficit. Note that the droplets considered in these early studies are very large compared to what is used (or at least desired) currently for propulsion applications. When large droplets are used, various modes of breakup are possible and these need to be considered.

Conceptual Models of Liquid-Fueled Detonations

As mentioned earlier, the work of Williams^{3,4} indicated that the structure of liquid-fueled detonations needs to be more complex than a shock wave followed by heterogeneous droplet combustion. Some combination of droplet deformation, breakup, evaporation, and burning is needed to account for the fact that detonations are observed in liquid fuels with a variety of droplet sizes.

Breakup Mechanisms in High-Speed Convective Flows

The atomization of a liquid jet and more specifically the breakup of large droplets is too complex a topic to be covered adequately in this paper. Selected works are emphasized based on their direct impact in helping us understand the observations made on liquid-fueled detonations. Ranger and Nicholls⁴⁵ reported on the breakup of 750- to 3000- μm droplets when subjected to the convective flow behind shock waves of Mach number 1.5–3.5 in air. They discussed the influence of various parameters on the rate of disintegration and on the time required for breakup to occur and formulated a model based on the droplet-stripping mechanism. Many other studies that followed this work have been discussed in the context of high-velocity convective gas flow behind shock waves by Fox and Dabora.⁴⁶ As they note, the “stripping mode” is expected to be the dominant form of breakup when the Weber number is higher than about 20. More recently, Pilch and Erdman⁴⁷ have summarized the various forms of breakup as a function of the Weber number.

Although most droplet breakup models are based on a single droplet in a uniform gas flow of infinite extent, in reality, the proximity of other droplets, as in a spray, will impact the breakup time.

For example, Fox and Dabora⁴⁶ showed that the breakup time is reduced even when a column of droplets is considered, due to the wake effects. Further studies by the same authors suggested that the breakup time in sprays can be 55–90% of that of an isolated droplet depending on the droplet spacing, the diameter, and the flow Mach number. Although there is uncertainty in these estimates, the droplet breakup models considered in current numerical simulations are relatively simple. This is an area that requires further study.

Impact of Droplet Breakup Processes on the Overall Detonation Model

Borisov et al.⁴⁸ included droplet breakup processes to extend the theoretical model of two-phase detonations. In addition to droplet evaporation, they considered both a droplet-stripping mechanism and a droplet deformation followed by breakup and came to the conclusion that evaporation and subsequent burning alone, without breakup, were still too slow for droplets greater than $10\text{ }\mu\text{m}$ in size to result in a steady detonation. Furthermore, the stripping mechanism resulted in such a long reaction zone that heat losses from that zone should lead to detonation failure. Thus, droplet deformation followed by breakup was needed to explain detonation in droplets on the order of $100\text{ }\mu\text{m}$. They note that propagation in droplets of about $1000\text{ }\mu\text{m}$ should be accompanied by local explosions at a relatively large distance behind the shock front. Part of the energy of this explosion is transferred to the shock front by secondary shock waves formed during the explosion. Shock waves moving in the opposite direction decrease the fraction of the total released energy supporting the detonation front. This provides an alternate account for the observed deficits in velocity.

Kauffman and Nicholls⁴⁹ continued the experimental studies with DECH droplets, focusing on the ignition of large fuel droplets in an oxidizing atmosphere. They observed combustion in the micromist that had been stripped from the parent drop and was entrained in the wake of the parent drop, confirming droplet stripping and subsequent burning as a viable mechanism for some liquid-fueled detonations. Combustion is not uniform but appears as a series of discrete explosions with the resulting shock waves interacting with the incident and bow shock waves. They also propose including the various delay times involved in droplet stripping, micromist evaporation, and chemical processes in an effective activation energy that would be dependent on the droplet diameter.

Pierce and Nicholls⁵⁰ emphasize the importance of considering the time-dependent nature of the flow in theoretical analysis, including both the forward- and rearward-moving waves generated by the explosive ignition of droplets after an “effective” induction period. The forward-moving blast waves accelerate the leading shock when they catch up with it. Between successive collisions of this kind, the leading shock is assumed to decay as it encounters new droplets. That is, the detonation velocity oscillates about a long-period average. By considering the droplets to be arranged in a simple cubic array—sheets or planes spaced apart—they are able to develop a consistent model to represent the oscillating flow. This appears to be the first explicit mention of the natural attenuation of the leading shock wave as it encounters new droplets.

An alternate model of spray detonations was proposed by Dabora,⁵¹ in which the perceived differences with gaseous detonations were emphasized. Unlike gaseous detonations where the energy release is continuous after an induction time, in a spray medium, “energy release occurs in a discrete manner at the site of the droplets.”⁵¹ This discrete nature is said to account for the blast waves originating from droplets that have been observed in experiments. These waves catch up to the main front and provide a means to couple the energy release with the shock front to maintain a steadily propagating wave. A schematic from their paper is shown as Fig. 2. Again unlike the gaseous case where the front “feels” the heat release in a continuous fashion, in a spray detonation, the coupling is with finite-amplitude waves. Therefore, he concludes that the blast strength must be sufficient to overcome the tendency of the shock front to decelerate as it moves through the droplets. He uses this information to derive a relation between the ratio of ignition delay to droplet breakup time and a heat release parameter.

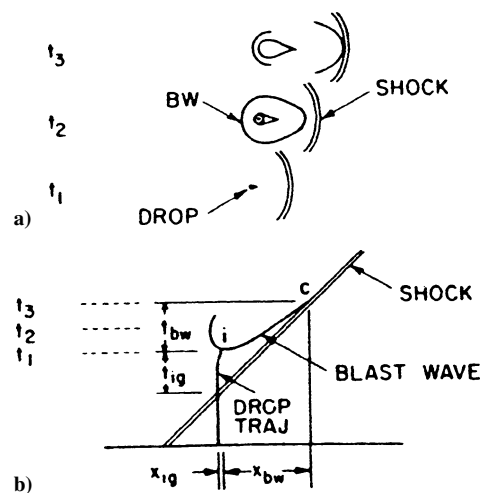


Fig. 2 Schematic showing the interaction between blast waves generated from the droplet and the shock front (from Ref. 51).

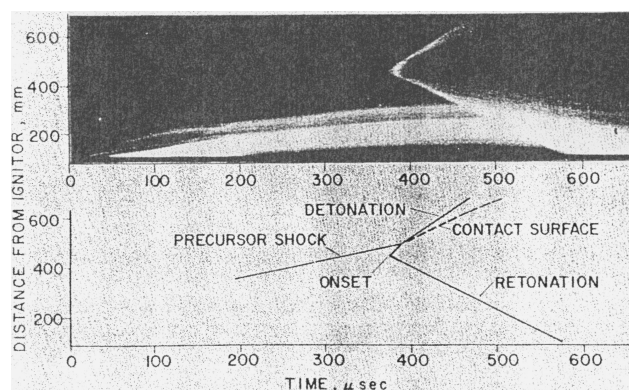


Fig. 3 Streak photograph and schematic showing the transition to detonation (from Ref. 53).

Based on their cylindrical detonation experiments in a pie-shaped shock tube, Bar-Or et al.⁵² report qualitative differences in the behavior of low-vapor-pressure (decane) and high-vapor-pressure (heptane) fuels. In the high-vapor-pressure case, a gaseous detonation was observed to propagate through the fuel vapor already present, followed by an extended region of droplet burning of the excess fuel. In the low-vapor-pressure case, long reaction zones and propagation rates appreciably below the calculated CJ value were observed. They propose a theoretical model that accounts for such differences in structure.

Effects of Droplet Size and Tube Diameter

The emphasis of the discussion so far has been on relatively large droplets ($>100\text{ }\mu\text{m}$) where a velocity deficit is observed in experiments and various conceptual models are proposed to account for this deficit. As the droplet size decreases, one should expect behavior more analogous to that of gaseous detonations. The well-known cellular structure of gaseous detonations and concepts such as the minimum tube diameter for sustained propagation should then be considered.

Unlike previous experimental studies, Bowen et al.⁵³ investigated detonation in decane fogs where the droplet size was estimated to be about $2\text{ }\mu\text{m}$. Thus, shattering, stripping, and other droplet breakup mechanisms could be neglected. A noteworthy observation from their work is that for such small droplets, the overall process of transition to detonation appears to be similar to that for gaseous detonations, as shown in Fig. 3, where a self-luminous streak photograph and its interpretation (both from Ref. 53) are shown. The figures suggest autoignition or “explosion within an explosion,” producing an overdriven detonation that propagates into the unreacted medium and a retonation that travels into the hot combustion products.

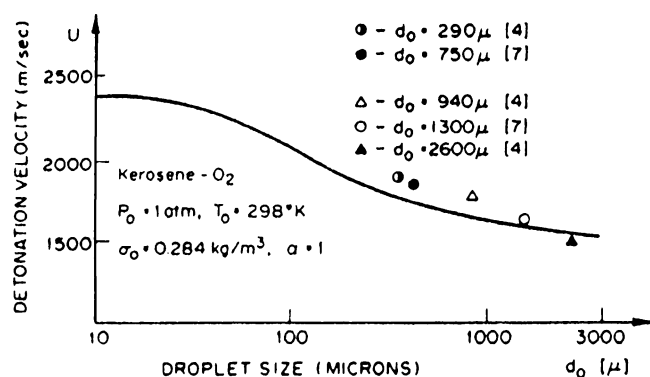


Fig. 4 Variation of detonation velocity with liquid droplet diameter (from Ref. 54).

However, even with the small droplets, steady velocities ($\pm 1\%$) are observed only from 2–12 m along the tube. Perhaps this is due to the relatively small diameter of the tubes considered.

They also varied the tube diameter from 0.49 to 2.22 cm and observed a strong dependence on the tube diameter, with higher velocities for the larger diameter tubes. This is perhaps because for the larger-diameter tubes, nearly self-sustained propagation might have been possible in these long tubes. Of some concern is their observation that “the detonation velocity may be up to 10% higher than the equivalent gaseous C-J velocity for lean mixtures.” No explanation has been offered but this could be due to inaccuracies in the estimation of stoichiometry of the mixtures involved and a poor estimation of the equivalent gaseous detonation velocities.

By the mid-1970s, the popular explanation for the observed velocity deficits was heat losses to the walls due to the long reaction zones needed in two-phase detonations, with some role also played by the rearward moving waves that are generated when the energy release occurs. Gubin and Sichel⁵⁴ proposed a new model where the observed velocity deficit is mainly due to incomplete fuel reaction rather than heat losses from the reaction zone. In this model, some of the fuel burns behind the C-J plane and hence does not have any effect on the detonation wave velocity. The amount of fuel that burns “effectively” is determined by the rate of disintegration of the liquid droplets and the ignition time delay. However, a limitation of the model is the assumption that the C-J plane is located at the place where ignition occurs (at the end of the induction zone). Furthermore, complete reaction (of the fuel formed in the breakup process) is assumed to occur instantaneously when ignition occurs. In spite of the limitations of the model, good agreement is obtained with experimental velocity data, as shown in Fig. 4. A noteworthy feature of the model is that the detonation velocity approaches the ideal C-J velocity for droplets smaller than 20 μm . This is an intriguing model that merits further study, with an independent determination of the C-J plane.

The dependence of observed detonation velocities and the velocity deficit on the tube diameter and droplet sizes for a variety of fuels has recently been summarized by Roy et al.²⁷

Detonation in Unconfined Fuel Clouds

Some of the observations made in initiating detonations in unconfined fuel-air clouds are discussed next. Bull et al.⁴² conducted experiments to study the initiation and propagation of spherical detonations in “unconfined” fuel aerosols (5–30 μm). As expected, it was more difficult to initiate spherical detonations than planar ones. This is also one of the few studies that provide detailed information on the method used to initiate the multiphase detonations. They used the method of overdriving with the blast wave from plastic high-explosive (PE-4) charges. Initiator charges of PE-4 (88% RDX) up to 0.5 kg were used. The energy content is estimated to be 4900 kJ/kg. As with planar detonations, a velocity deficit is observed, but this occurs even with relatively small droplets. The velocity with a highly volatile fuel (hexane) is about 1580 m/s (6–13% below C-J) for droplets of 6–17 μm . The deficit was larger for droplets

of 50–90 μm , with these droplets having a velocity of 1300 m/s. It is interesting to note that a velocity deficit is observed even without any heat losses to confining walls (because these are essentially unconfined). With low-vapor-pressure fuels (dodecane and decane) detonations could not be initiated with the initiator charges tried. They conclude that with these fuels, a certain quantity of fuel vapor might have to be present for detonation to occur in droplets bigger than about 10 μm . This appears to be the first clear indication of the importance of the presence of fuel vapor for initiation of multiphase detonations in air. It also confirms that velocity deficits can occur even without any losses to walls (because these are unconfined detonations).

Several other papers^{44,55,56} have emphasized the dependence of the detonation properties on the fuel vapor content. Alekseev et al.⁴⁴ enhanced the detonability of kerosene sprays with the addition of gasoline, a high-vapor-pressure fuel. However, even a higher-vapor-pressure fuel such as gasoline does require some time to vaporize and saturate the mixture. To determine the effect of the quantity of gasoline vapor on the detonability, they varied the ignition delay from a minimum of 0.8 s to a maximum of 4 s. They found that waiting for more than 1.7 s had no effect on the detonability and little effect on the minimum energy required for initiation. They also observed oscillations in the leading shock velocity for kerosene-air mixtures, with drops in velocity down to 700–900 m/s. The period of oscillations was about 2–3 s. The average velocity was 1000–1300 m/s. They suggested that these oscillations could be due to “a near-limit transversal dimension of the cloud.”

Cellular Structure of Liquid-Fueled Detonations

Detonations in a very volatile fuel with small droplets should have characteristics very similar to those of gaseous detonations. However, the situation is unclear for less volatile fuels at room temperature.

The primary emphasis of the work of Papavassiliou et al.⁵⁶ was on measurements of the cellular structure of detonations in a low-vapor-pressure fuel (decane) mixed with nitrogen and oxygen. They studied detonations in both heterogeneous and homogeneous mixtures by controlling the initial temperature of the mixture. The droplet size was 5 μm for the heterogeneous case (tube at 25°C). Homogeneous mixtures were obtained by heating the tube (to 100°C or 185°C) and letting the mixture sit under heated conditions for 30 min. For all cases, the initial pressure was 1 atm. Hence, the density is lower for the heated tube cases, because some venting was allowed to keep the pressure constant. The vertical detonation tube was 64 mm in diameter and 3 m in length. Ignition was with a powerful spark (120 J of stored energy) and a 50-cm-long Shchelkin spiral was also used to aid in the transition to detonation.

Several key observations were made in this study.⁵⁶ Successful initiation and stable self-sustained propagation were observed even at 25°C (heterogeneous mixtures) for a range of mixture stoichiometries in decane-oxygen mixtures. The agreement with calculated C-J velocities for the equivalent gaseous mixtures (see Fig. 5) was said to be very good (within 10%), although there seems to be a deficit for very lean mixtures. The detonation pressure ratio (Fig. 6) was generally lower, though mostly similar to the gas-phase values. For the heated tube (vapor-phase decane detonations), the cell size was similar to that for the alkane group (ethane, propane, and butane). For the cold tube (5- μm droplets), the cell size was larger by a factor of 2. Because the initiation energy is roughly proportional to the cube of the cell size, an order-of-magnitude increase in initiation energy is required even with 5- μm droplets. They suggest that this effect accounts for the difficulty in detonating unconfined decane-air mixtures. This also appears to be one of the few studies of liquid-fueled detonations that have dealt with the cellular structure. With the increase in cell size with decrease in temperature and fuel-vapor content, one wonders how many of the early observations on liquid-fueled detonations have been influenced by the use of tube diameters smaller than an effective detonation cell size. However, it must also be remembered that the concept of a detonation cell and the multiple shock structure, although well established in gaseous mixtures, is not yet clear in low-vapor-pressure liquid-fueled detonations.

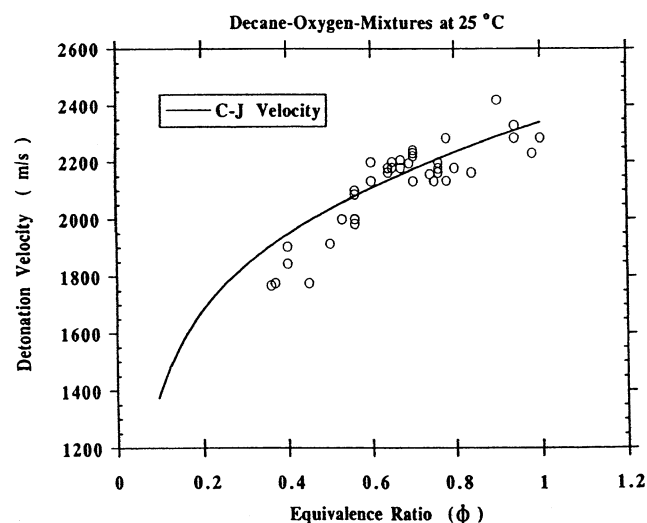


Fig. 5 Comparison of measured detonation velocities in decane-oxygen mixtures at 25°C and computed C-J velocities for a range of equivalence ratios (from Ref. 56).

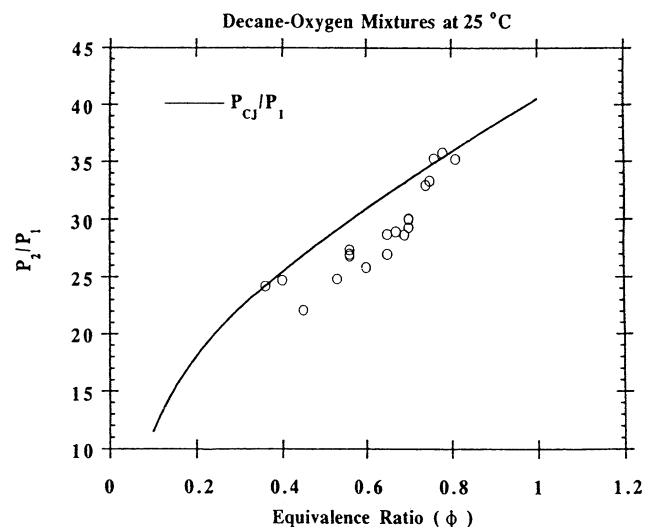


Fig. 6 Comparison of measured detonation pressure ratios in decane-oxygen mixtures at 25°C and computed C-J pressure ratios for a range of equivalence ratios (from Ref. 56).

Initiation and Detonability

Minimum initiation energy of direct detonation initiation by a powerful source is usually considered to be a measure of mixture detonability. As discussed previously, the difficulty of initiating detonations in heterogeneous fuel-air mixtures is decreased if some fuel vapor is present. This can be achieved in practice by heating the tube.

Several papers appeared in the early 1990s focusing on the ignition and detonability of multiphase mixtures.^{43,44,56–58} Boiko et al.⁵⁷ investigated shock-induced combustion of tridecane, kerosene, and diesel fuel drops in air at various pressures and shock strengths through the use of a shock tube. The work provided quantitative information on the time and length scales required for combustion to occur after the passing of the incident shock wave for many experimental conditions. Unfortunately, the study investigated drop sizes larger than 1 mm and revealed that the heat release was largely decoupled from the shock wave. Dabora⁵⁸ investigated the effects of adding propyl nitrate and butyl nitrite on the detonability of a kerosene spray. This study also utilized large droplets, which again showed signs of decoupling the heat release from the shock wave.

In the past 5 year there has been renewed interest in multiphase detonations in tubes because of their application to pulse detonation

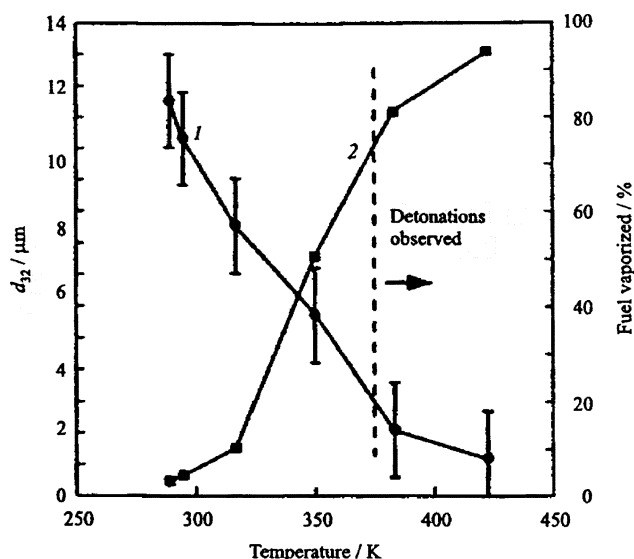


Fig. 7 Sauter mean diameter (1) and percentage of fuel vaporized (2) as a function of PDE inlet temperature for a JP10-air mixture (from Ref. 12).

engines. The problems that must be overcome and the progress that has been achieved to date in the use of liquid JP-10 in pulse detonation engines have been reported in a series of papers by Brophy et al.^{10,12,14} Their initial work¹⁰ dealt with characterization of the atomizers used and successfully initiating detonations in JP10/O₂ mixtures with droplet diameters predominantly below 10 μm . The detonation velocities observed were close to the C-J values, except for some lean mixtures. Even in this case, the deficit was only about 10%. The observation is again made that in a two-phase flow, the fuel must be significantly vaporized before a substantial reaction can occur. Therefore, in a subsequent study,¹² the fuel was preheated using various inlet temperatures. Corresponding to each temperature, the particle size and amount of vapor were estimated. Fig. 7, from Brophy et al.¹² shows the variation in the Sauter mean diameter (SMD) and percentage of fuel vaporized as functions of temperature. In addition, the conditions under which detonations were observed are also marked in the figure. The figure shows that under the conditions of the test, JP10/air detonations occur for droplet SMD values of about 3 μm and for an estimated fuel-vapor content of about 70%. The inlet temperature corresponding to these conditions is 375 K. At 425 K, the fuel will be completely vaporized. For the cases in which detonation occurred (375 to 425 K), the observed propagation velocities were within 2% of the C-J values. Thus, laboratory PDEs operating with JP10 in both oxygen and air have now been demonstrated.

Schauer et al.²⁰ have reported successful operation with both partially and fully vaporized liquid fuels in their multicyle, multitube PDE. Initiation and operation with liquid fuels may be easier during multicyle operation²² because the tube will be warm, inducing vaporization of the liquid fuel. Injecting the fuel into a mixing zone and preheating it is another approach to easing the initiation and transition to detonation.

The detonability of a variety of fuels in a 36-mm-diam, 7-m-long tube has been assessed recently.¹⁹ For each fuel that detonated, the oxidizer-to-fuel ratio was varied until a separation of the shock wave from the flame front and a sharp decrease in the detonation velocity were observed. It is acknowledged that the concentration limits obtained using this method will change for wider and longer tubes using stronger ignition sources. However, the results do highlight the narrow range of parameters over which detonation is observed in liquid fuels.

Another approach for varying the amount of fuel in liquid form was investigated by Knappe and Edwards.²¹ In their experiments, they investigated detonations in mixtures of gaseous propane and liquid decane and varied the amount of fuel present in the liquid phase from 0 to 100%. The oxygen content was varied from 60 to

100% and the SMD of the droplets was varied from 16 to 28 μm . The detonations in these test mixtures were initiated by an ethylene-oxygen detonation wave, which itself was initiated by a plasma jet. When the oxidizer is 100% oxygen, the detonation velocity systematically decreases as the amount of liquid fuel is increased from 35 to 100%. When nitrogen is present, the trend is not as clear because the impact of nitrogen dilution seems to be greater on propane than on decane. The effect of the mean droplet diameter (over the narrow range investigated) on detonation velocity is observed to be relatively minor in oxygen mixtures, becoming more important as the amount of nitrogen is increased.

Reducing the initiation distance and the amount of energy required for initiation are key challenges in the development of propulsion systems based on detonation. Promising results have been obtained in a recent comprehensive study^{18,24} using controlled triggering of electrical discharges. The effects of discharge time, shape, and location as well as of number of discharges and tube parameters were all investigated. Relatively small droplets (mean diameter of 5 μm) of a volatile fuel, *n*-hexane, was considered. Still, at the first discharge location, the fuel was mostly in droplet form, whereas, at the second location (20 cm downstream), it is likely to have been mostly in vapor form.²⁴ With two discharges and optimal delay time between the discharges, the initiation energy can be considerably reduced. Addition of a Shchelkin spiral results in further reduction in the initiation energy required and widens the range of timing parameters, resulting in a more robust operation.

Numerical Simulations

Numerical simulations of liquid-fueled detonations are far fewer than those of gas-phase or gas-particle detonations. Burcat and Eidelman⁵⁹ and Eidelman and Burcat⁶⁰ conducted numerical simulations of a detonation wave in a cloud of heptane droplets and were able to separate out the numerical oscillations from the physical ones. Their simulations captured the secondary waves emitted by the droplet combustion and its propagation forward to reinforce the leading shock front. They considered droplet radii ranging from 50 to 500 μm and found that the detonation velocity is inversely proportional to the width of the reaction zone behind the shock front. Interestingly, they observed a velocity deficit (when compared to the expected C-J velocity) only for droplets larger than about 100 μm in diameter. This is perhaps due to the simplified submodels used to represent the multiphase and chemical effects in their simulations.

The work of Zhdan⁶¹ and Voronin and Zhdan⁶² has focused on simulating the initiation of heterogeneous detonations. They have considered initiation both using a condensed explosive⁶¹ and using gaseous detonation in a stoichiometric hydrogen-oxygen mixture.⁶² Calculations show that the heterogeneous detonation ceases when the length of the induction zone exceeds the distance from the shock wave front to the point of droplet disintegration. For a low-volatile fuel, heptane, self-sustained detonation is observed in oxygen, but not in air.

More recently, Vasil'ev et al.⁶³ have reported on the initiation of detonations in heterogeneous systems using a comprehensive model where the detonation wave consists of a lead shock wave followed by a relaxation zone where processes such as acceleration of the droplets, their deformation and possible breakup, phase transition, convection, diffusion, and chemical reaction take place. Detonation initiation in monodispersed and polydispersed sprays of liquid fuels in air and oxygen with a range of droplet sizes from 50 to 700 μm were considered. The results of these simulations have been used to develop simple models and analytical formulas for estimating the initiation energies for planar, cylindrical, and spherical geometries.

In another study, Zhdan and Prokhorov⁶⁴ reported what may be the first observation of cellular structure in the numerical simulation of a cryogenic hydrogen and oxygen mixture. The calculated cell size increased almost linearly with increase in the initial diameter of oxygen droplets.

Law et al.¹⁵ conducted steady state, one-dimensional analysis of heptane-air spray detonations using detailed chemistry in addition to accounting for droplet heating, vaporization, and drag effects. They also considered the effect of wall drag and heat losses within

the framework of a one-dimensional analysis. An interesting observation from their analysis was the existence of an optimal droplet size for faster detonation velocities and wider quenching limits.

Chang and Kailasanath [16] showed that the well-known attenuation of shock waves by a dispersed phase is increased when droplet breakup and vaporization effects are included in the simulations. Therefore, to establish a liquid-fueled detonation, the effects of energy release must continually overcome the attenuation effects. This suggests that the effective induction distance (before significant energy release) must be short for the pressure waves generated by the energy release to travel forward, couple with the shock front, and create a sustained detonation wave.

Cheatham and Kailasanath^{23,25} extended these studies to include various choices of droplet drag and convective-enhancement submodels. It was found that the uncertainties in such models, although significant in shock-attenuation studies, are secondary in detonation studies due to the overwhelming effect of the chemical energy release. Attention was focused on relatively small droplets to minimize droplet breakup effects and the length of the tube was also limited to 1.5 m to make the results more relevant to propulsion systems. For the small range of sizes considered (2.5 to 20 μm), the shock-to-detonation transition and attainment of a self-propagating detonation (in the context of a one-dimensional model) took a longer time for the larger droplets. Small velocity deficits, when observed, could be attributed to incomplete reaction due to inhomogeneity of the fuel-oxygen mixture. Even for the small range of sizes, the size of the reaction zone, the overall structure, and the location of the sonic point all varied, indicating the need to examine this problem further, including the multidimensional structure and dynamics.²³ Prevaporization effects were isolated from droplet size effects by considering various mixtures, initially at two-phase equilibrium at a series of initial temperatures.^{23,25} The results indicated that smaller droplets and higher levels of heating and prevaporization result in a smoother and faster transition to self-sustained detonation, as shown in Fig. 8. Here, the shock-front velocity in a stoichiometric JP10-oxygen mixture is shown at a series of locations along the tube for five cases. In all cases, steady detonation is initiated in a fully vaporized, gaseous mixture at 455 K that fills a small section of the tube. The remaining section of the tube is filled with a gaseous mixture, droplets of diameter 10 or 20 μm at 298 K, or a combination of 20- μm droplets and vapor at 308 or 323 K. For the gaseous case, the detonation front continues at the C-J detonation velocity of 2300 m/s down the remaining section of the tube. For all other cases, as expected, the front velocity decreases when the droplets are encountered. Only for the smaller droplet case (10- μm droplets initially at 298 K) or the case with a greater amount of prevaporization (20- μm droplets initially at 323 K) does the velocity approach the expected C-J detonation velocity by the end of the tube.

The work was extended to fuel-air mixtures and the impact of the observations on single-cycle performance of a pulse detonation

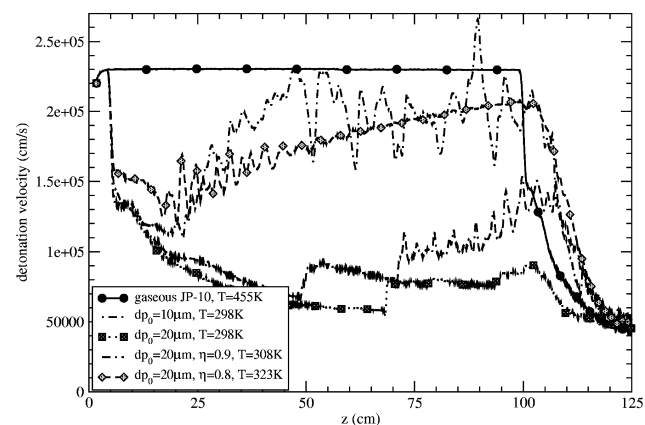


Fig. 8 Effect of prevaporization and droplet size on the shock-to-detonation transition in a stoichiometric JP10-O₂ mixture (from Ref. 25).

engine has been assessed²⁵. Similar levels of performance are attained as long as the detonation is fully developed by the end of the tube. However, this requirement imposes stricter constraints on the droplet size and degree of prevaporization for JP10–air mixtures compared to JP10–oxygen mixtures.

Conclusions

Although our understanding of multiphase detonations is clearly less developed than for gas-phase detonations, several general observations can be made from the brief review presented. Theoretical, computational, and experimental studies have shown that if the spray droplets are fine enough (less than about 10 μm), detonations propagating at about the equivalent gas-phase detonation velocity can be attained in a variety of fuel–oxygen systems. Detonations are indeed observed in multiphase mixtures with much larger droplet sizes (even on the order of millimeters). This is usually reconciled by the observation that the larger droplets are reduced to smaller ones and vapor by a variety of droplet breakup mechanisms, including shattering and stripping. In general, the propagation velocity observed in these cases is below the equivalent gas-phase velocity. Wall losses, incomplete combustion before the C-J plane, and energy loss due to rearward propagating waves have all been proposed as reasons for the observed velocity deficits. Theories based on these hypotheses have had some success in explaining particular experimental observations. In the opinion of this reviewer, none of these mechanisms have been conclusively established and this is a topic that needs additional research.

In many cases, the droplet breakup behind the lead shock wave might occur rapidly enough to leave behind a heterogeneous mixture of fine droplets and fuel vapor in an oxidizing atmosphere. The details of the heterogeneous combustion of this mixture and the impact that it can have on the structure and propagation of the detonation wave have not been understood and are a topic worthy of detailed study.

The amount of energy required to initiate detonations in gaseous mixtures has been strongly correlated with the observed cell size. The difficulty in initiating detonations in many hydrocarbon–air mixtures has been alleviated by heating the fuel–air mixture, which results in a reduction of the cell size. Although the cell sizes of liquid fuel–air mixtures have not been established, a similar approach helps in the initiation. In the case of liquid fuel–air mixtures, heating also results in partial vaporization of the droplet and reduction in the droplet size, factors that certainly aid in the initiation and propagation of detonations. In the presence of air (rather than oxygen), the minimum droplet size required to support detonations without any velocity deficit is smaller, or equivalently, the amount of vapor present must be larger.

The emphasis in the past has been on the final velocity observed in multiphase detonations. For propulsion systems such as the PDE, the actual distance required for transition to detonation is an important factor placing additional constraints on system configurations and performance. In addition, injection of fuel sprays usually results in considerable wall deposition. Although detonations have been successfully initiated in wall films, the propagation velocity observed has been significantly below the C-J value. The quantitative impact of the velocity deficits and the additional distances involved in transition to detonation on the performance measures of a PDE have not yet been ascertained. This brief review emphasized the need for further studies of multiphase detonations, including their multidimensional structure, with emphasis on their impact in the operation and performance of detonation engines.

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