Experimental Implementation of a Converging Diverging Nozzle Technique to Study Shock Reflections in Reactive Gases

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1 Introduction

Detonation waves in gases are very unstable and form a dynamic cellular structure on the wave front. The complex phenomena occurring at the cellular front are believed to have an important influence on the bulk reaction rates of the wave and the detonability of a mixture [1, 2]. Nevertheless, the structure of the detonation front is still very poorly understood and predicted. This is due to the complex phenomena occurring within the detonation structure, comprised of shock reflections, hydrodynamic turbulence and rapid exothermic reactions among hundreds of chemical species. Experimental observations of the flow fields within the cellular structure are typically limited to single images of the reaction structure and chemical species (see for a recent review [3]). The inherent variability in the detonation cellular structure does not allow a proper interpretation of these results for irregular structures. Due to its innate multi-scale transient character, direct numerical simulations in three dimensions are also not currently possible.

It is thus desirable to develop an experimental technique that can permit the study of triple shock reflections in reactive gases, and the accompanying dynamics of the exothermicity in a reproducible fashion. The experiment would thus minimize the intrinsic stochasticity of self-sustained detonations and permit well-defined initial and boundary conditions, conducive to modelling. Some time ago, a technique was suggested by White and Cary to generate laminar detonations [4] which can then be subjected to shock reflections in a reproducible manner. The technique consists of passing a self-sustained detonation through a converging-diverging nozzle. Figure 1 shows a numerical demonstration of the technique. In the converging part, the detonation becomes overdriven, while in the diverging part, the detonation may locally decouple into a shock followed by a reaction wave [5]. It is this attenuated quasi-one-dimensional wave that can be further subjected to reflections, in order to generate triple shock reflections, as demonstrated by White and Cary [4].

The present study is an implementation of White's nozzle technique to study shock reflection in reactive gases and the ensuing exothermicity. We first provide the scaling laws that permit the generation of the quasi-onedimensional waves in a broad range of reactive mixtures, and identify the conditions that can isolate either reactive or non-reactive shock reflections. We conclude by studying the ignition phenomena in methane-oxygen detonations, which have been observed in the past to exhibit wider detonability limits [1,2] and enhanced ignitability [6] compared with predictions based on current thermo-chemical data [7].



Figure 1: Simulation of detonation failure over a Converging-Diverging nozzle

2 Experimental Technique

The experiments were conducted in a thin rectangular channel, illustrated in Figure 2. The detonation tube consists of a 3.5 meter long rectangular channel, 203 mm high and 19 mm wide. It is separated into three sections of equal length. The first section is used as the initiating driver, where oxy-acetylene is used. The driver gases are initially separated from the test gases by a thin plastic diaphragm. The detonation, initiated in the driver section, is transmitted to the test mixture, in which a self-sustained detonation is rapidly initiated. Pressure transducers located along the shock tube length monitor the detonation wave strength. All gas mixtures studied were prepared by the method of partial pressures in a separate pressure vessel, and left to mix diffusively for 24 hours before the tests. In all experiments, the tube was first evacuated to pressures less than 100 Pa before filling with the test mixture.



Figure 2: Illustration of the shock tube

The walls of the third section of the shock tube are made of optical quality glass, which permitted us to conduct detailed flow visualization using the Schlieren technique. The Schlieren optical system is a conventional Z set-up using two parabolic 318mm diameter f8 mirrors manufactured by Edmund Optics. For the light source, a two-spark gap flash system (Palflash 501, Cooke Corporation) was used, which permitted us to obtain two consecutive spark discharges with arbitrary time delays and microsecond resolution. Each flash duration was less than 1 microsecond. The two consecutive flashes were used to generate two separate Schlieren images, captured with a PIV camera (PCO.2000, Cooke Corporation).

The converging-diverging nozzle used to implement White's technique consisted of a triangular obstacle made of Delrin, where the upstream ramp angle was 15° and the downstream angle was 30° . The latter was chosen to simulate the incidence angle of shock reflections in cellular gaseous detonations [8]. Two nozzles were tested, with throat dimensions *b* of 2 mm and 19 mm.

3 Experimental Results

For a given reactive mixture, two different outcomes were observed at the exit of the nozzle. For sufficiently high initial pressures, that is, sufficiently sensitive mixtures, a self-sustained detonation wave was observed in the diverging section. An example is shown in Figure 3. Below a critical pressure, however, the detonation decoupled into a shock-reaction zone complex and continuously decayed in strength. An example is shown in Figure 3.

The critical conditions for direct transmission are reported in Table 1. Also listed is the correlation between the throat dimension b and the cell size of the mixture λ , obtained from previous experimental correlations [9–12]. The results can all be correlated approximately by $b \approx \lambda$, which can be used in the future as an initial guideline to implement White's experiment.

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Figure 3: Decoupled shock reaction zone complex a stoichiometric CH_4+O_2 mixture at 6.9 kPa (A) and a diverging detonation at 17.9 kPa at the exit of the *b*=19mm converging-diverging nozzle.

Mixture	Po [kPa]	Critical Factor (b / λ)	<i>b</i> [mm]
$C_{3}H_{8}+5O_{2}$	11.0	0.18	2
$2C_{2}H_{2}+5O_{2}$	4.0	0.50	2
CH_4+2O_2	17.9	0.95	19
$2H_2+2O_2$	13.1	1.93	19

Table 1: Critical conditions for detonation transmission in the converging-diverging nozzle

It was found that the dimension of the throat permitted further control of the strength of the decaying wave as it encountered the compression corner at the bottom of the ramp. It also permitted us to monitor the separation between the leading shock, and the following reaction zone. An example is shown in Figure 4 in a mixture of $C_3H_8+5O_2$ initially at 10.3 kPa, using a throat size of 2 mm. As can be seen, the reaction zone is now far from the lead shock. The image was acquired as the leading shock reflected off the bottom wall, giving rise to a Mach reflection. In this case, no exothermicity was observed behind the Mach shock. The technique thus permits the study, quite effectively, of the structure of Mach reflections in reactive gases, without the exothermicity affecting the flow field in the reflection process.

The effect of exothermicity on the shock reflection process was studied in the methane-oxygen mixture with the 19 mm throat nozzle. Figure 5 shows the Mach reflection process when the gas behind the Mach shock has not yet ignited at an initial pressure of 17.6 kPa. In this photograph, the Mach shock has a Mach number of approximately 3.4. The photograph clearly shows the double Mach reflection occurring near the bottom wall. It also shows the refraction of the reflected shock at the reaction zone, separating the shocked and unreacted gases from the reacted gas.

At a slightly higher pressure of 17.9 kPa, approaching the critical conditions for detonation transmission (see Table 1), we observed re-ignition behind the Mach shock, as shown in Figure 6. As can be seen in the photograph, the gas behind the Mach shock has now reacted and a very thin reaction zone is apparent behind the Mach shock. Similar flow fields have been observed by Radulescu et al. [2]. Note how the transverse shock has the typical refraction pattern at heavy-to-light density interfaces. It is also interesting to note that the un-reacted gas layer shocked by this transverse wave acquires a very fine texture, potentially through Richtmyer-Meshkov instability.



Figure 4: Mach reflection in C_3H_8 +5 O_2 at the exit of the b = 2 mm nozzle at 10.3 kPa



Figure 5: Double Mach reflection in CH_4 +2 O_2 at the exit of the b = 19 mm nozzle at 17.6 kPa

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Figure 6: Double Mach reflection in CH_4+2O_2 at the exit of the b = 19 mm nozzle at 17.9 kPa, leading to ignition behind the Mach shock

In the experiment shown in Figure 6, the incident shock strength prior to the reflection has a Mach number of approximately 2.8. Using shock-polar analysis, the strength of the Mach shock is readily determined, yielding in this case a Mach number of 3.9 for the non-reactive Mach shock. Using methane-oxygen thermal data, the state behind the shock yields a pressure of 3.3 bar and a temperature of 940K. The ignition delay of the methane-oxygen mixture, obtained with the GRI3 kinetic mechanism [7] in constant volume calculations using Cantera [13], is approximately 0.3 seconds. This is approximately 3 orders of magnitude longer than the time of ignition observed in the experiments.

This very large discrepancy in the ignition characteristics of methane-oxygen echoes the findings of Radulescu et al. [2], who also found that methane-oxygen detonations react much faster across the detonation wave structure than predicted via hydrodynamic simulations. Similar ignition discrepancies have also been noted by Gardner [6], in a shock tube study of ignition of methane-oxygen-argon mixtures.

At present, it is unclear whether the source of this discrepancy is due to faulty chemical kinetics of methane at low temperatures [6], or novel physical phenomena not properly accounted for in the shock reflection process at the detonation triple points. For example, the estimate above ignores any viscous dissipation in the forward jet accompanying this type of double Mach reflection [8]. It also ignores any dissipation in the viscous boundary layers, which would also generate larger temperatures. Although the present experiments do not provide an answer to this question, they provide the experimental framework by which such questions can be answered in the future by comparison with detailed numerical models. This comparison is facilitated by the well-posedness of this shock reflection ignition problem.

4 Conclusions

The implementation of White's technique to study reproducible shock reflections in reactive gases permitted us to isolate the anomalous ignition of methane-oxygen detonations, previously reported to ignite much more readily

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than can be currently predicted [1, 2, 6]. The well-posedness of the present experimental technique may be conducive to comparison with detailed models in the future in order to address this anomalous ignition phenomenon.

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