Advances in Shock Tube Techniques for Fundamental Studies of Combustion Kinetics

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1 Introduction

Shock tubes can provide well-defined temperatures and pressures for combustion kinetics investigations that cover broad regimes of engineering and scientific interest. Shock tube experiments can be performed at temperatures of 500-5000 K (and higher) and pressures from sub-atmospheric to 500 atm (and higher). Measurements performed behind reflected shock waves have near-instantaneous heating times, spatially uniform mixtures, and occur in near-stationary (stagnant) flows. However, advances in the understanding of combustion kinetics have led to the need for even higher quality experimental data for model validation and refinement. This need for higher quality experimental data has provided new challenges for shock tube experimenters. Shock tube performance and models must be improved; shock tube operating regimes must be extended; real fuels must be studied; and sensitive species-specific diagnostics must be implemented. And good progress towards these goals is taking place. In this presentation, we overview work in several of these areas.

2 Achieving Uniform Pressure and Temperature

Many combustion processes are strongly temperature or pressure sensitive. Measurements of ignition delay times with large activation energies or strong pressure dependencies, for example, are very sensitive to post-shock temperature and pressure variations in test facilities. Conventional shock tubes will generally have some systematic variation in pressure and temperature as a consequence of the practicalities of developing shocked flow in long tubes. However, it is possible to reduce (and in some cases effectively eliminate) these variations by the addition of driver-section inserts.

To our knowledge, Dumitrescu [1] was the first to propose the idea of modifying the shock tube by inserting a properly designed cone-shaped obstacle into the driver section of a shock tube, as a means of generating more-constant reflected-shock conditions. Expansion waves reflected from the surface of the driver insert continuously propagate downstream into the driven section. The gentle decrease in pressure caused by these expansion waves is superimposed on the slow pressure rise related to the boundary layer growth. When the two opposing pressure changes are of the same magnitude, the boundary layer effects on temperature and pressure of the region behind reflected shock waves can be effectively eliminated, leading to a more-constant reflected shock pressure. The effect on the

reflected-shock test gas pressure when an insert designed using this method is employed is illustrated in Fig. 1. See (18) for details.



Figure 1. Example of the effect of driver inserts on reflected-shock pressure profile. Driver gas mixture: 50% N₂, 50% He; driver section length 3.3 m. Driven gas argon; driver and driven section diameter = 14.3 cm; driven section length = 8.5 m. Initial reflected shock conditions: ~ 900 K, 4 atm. dP/dt without driver insert: 1.7%/ms; dP/dt with driver insert: 0%/ms.

3 Extending Test Times

There is currently strong interest in low temperature hydrocarbon kinetics, in particular, to study the role of oxygen addition chemistry in the negative temperature coefficient (NTC) regime. To study the combustion processes that occur in this regime (which are slower than at high temperatures), longer test times at lower temperatures are needed. Conventional shock tubes with short driver sections (~3 meters) and long driven sections (~8 meters) (developed primarily for experiments at higher reflected shock temperatures) typically have relatively uniform temperatures and pressures only over test times of 1-3 ms at these lower temperatures. These test times are limited generally by one of two phenomena. The first phenomenon is the arrival of the expansion wave from the driver section of the shock tube, which isentropically cools the test gas. The second limiting phenomenon is the arrival of backward-propagating waves from reflected shock wave-contact surface interactions, which can modify the test gas temperature and pressure.

The first of these phenomena, the arrival of the expansion wave from the driver end wall, can be delayed significantly by extending the length of the driver section. In our facilities we have increased this length to approximately 12 meters. This delays the arrival of the driver expansion wave at the driven-section end wall, giving an available test time with nitrogen driver gas of approximately 35-40 ms and we have achieved test times up to 100 ms at certain conditions. The second of these phenomena, the reflected shock wave-contact surface interaction can be minimized (or eliminated) if a "tailored" driver mixture is used. See Nishida for a theoretical analysis of tailoring [2]. The tailored driver mixture has the property that the coefficient of reflection for the reflected shock wave is zero at the contact surface between the test gas (usually argon or air) and the driver gas (normally helium, but in the case of tailored driver gas mixtures typically a helium/nitrogen or helium/argon mixture).

The ability to extend shock tube test times to 10's of milliseconds enables the experimenter to directly compare shock tube and RCM (rapid compression machine) and FR (flow reactor) measurements at similar thermodynamic conditions. RCMs and FRs have generally been sources of ignition delay data for longer test times, needed for low temperature studies, but with limited upper temperature and

pressure range capabilities (because of heating and material constraints) and with larger uncertainties associated with fluid mechanics (RCM) and mixing times (FR). Generally, shock tubes have been the accepted source of kinetics data for short reaction times, e.g. < 10 ms, and hence high temperatures, while RCMs and FRs have been the accepted approach for longer test times, e.g. > 10 ms. The shock tube facility upgrades noted above enable the test time limit of shock tubes to overlap with these other approaches and thereby provide complementary reaction data.

3 Aerosol Shock Tube and Low Vapor Pressure Fuels

Current interest in the chemistry and high-temperature behavior of low-vapor-pressure liquid fuels (such as jet and diesel fuel) has motivated an effort to extend current shock tube techniques to enable study of these fuels. Many existing methods to measure low-vapor fuels have technical drawbacks. Shock tube and mixing facility heating to raise the fuel vapor pressure increases the chances of fuel cracking, incomplete evaporation, surface reaction, or low-temperature oxidation. The use of diesel injectors to load the shock tube with spray droplets of fuel produces a highly non-uniform distribution of fuel and stoichiometries and convolutes the evaporation and ignition delay time.

To avoid these technical difficulties, an aerosol shock tube can be used [3]. There are three major steps in the operation, see Fig. 2. First, the shock tube is uniformly filled near the end section with a micron-sized aerosol fuel/oxidizer carrier gas mixture. Second, this mixture is heated and fully vaporized by the passage of the incident shock wave. Third, the ignition experiment is performed in the fully evaporated test gas mixture behind the reflected shock wave.



Figure 2. Schematic of aerosol shock tube showing the three-step operation.

The advantage of the aerosol shock tube in providing purely gas-phase ignition delay times can be seen in the area of diesel fuel ignition. The aerosol shock tube provides ignition delay times for *gas-phase* diesel fuel that are more readily interpretable. Many early measurements of diesel ignition delay times include both the time for evaporation and the time for chemical reaction, or suffer from varying varying stoichiometry throughout the measurement volume because of both the droplet size distribution and the variation of this distribution and loading in the spray cone.

4 Constrained Reaction Volume Strategy

The constrained-reaction-volume (CRV) strategy is a new method that has been applied successfully for conducting reflected shock experiments at near-constant pressure, by reducing pre-ignition pressure rises due to combustion heat release, as well as avoiding remote ignition. Instead of filling the entire driven section with test gas as is done for a conventional-filling experiment, the test-mixture is filled into the driver section and compressed by a non-reactive gas to the endwall of the shock tube. This limits the volume of test gas mixture in the shock tube and thus limits the pressure excursions that occur during ignition. Figure 3 demonstrates that the pressure time-history for an ignition experiment is almost identical to a non-reactive experiment. Further details may be found in [4].



Figure 3. Pressure trace of a CRV ignition delay time experiment for ethylene/O₂/Argon. Reflected shock conditions: 1130 K, 1 atm, 0.4% C₂H₄/O₂/argon, ϕ =0.3.

5 Species-Specific Laser Diagnostics

In our laboratory, we have developed over the past 25 years, cw (continuous wave) narrow-linewidth, highly-sensitive, laser absorption diagnostics for a wide variety of combustion-relevant species. Quantitative measurements can be made for fuel (at 3.39 microns), transient radicals such as OH (at 306 nm and CH₃ (at 216 nm), stable intermediates such as C_2H_4 (at 10.5 microns) and CH₄ (at 3.17 microns) and combustion products such as CO (at 4.6 microns), CO₂ (at 2.7 microns) and H₂O (at 2.5 microns). Recent developments in tunable diode lasers have opened up many new wavelength ranges and enabled laser absorption probes for many new species in the infrared. In particular, measurements of acetylene (at 3.0 microns) and iso-butene (at 11.3 microns) are now possible.

6 Imaging Methods

Current shock tube combustion experiments generally assume that the test environment behind a reflected shock wave is quiescent and that ignition processes progress uniformly over the entire test volume. However, various past investigations, mostly based on schlieren data, have observed non-uniform ignition in certain test regimes. Using conventional diagnostics (pressure, emission, and laser absorption), a high-speed chemiluminescent imaging system, and a CRV shock tube filling strategy, we have begun to study the ignition of combustion systems with long ignition delay times. Our goal is to map the boundary of this uniform and non-uniform ignition behavior in our imaging shock tube and ultimately to develop strategies and facility refinements to minimize non-ideal effects.

Images through the endwall of the shock tube of OH* emission were acquired with a Phantom v710 CMOS camera using a 12 kHz acquisition rate, with a typical resolution of 200 μ m per pixel. Conventional sidewall OH* emission, and fuel concentration time-history measurement using 3.39 micron HeNe laser absorption were also performed.

Figure 4 shows a 986 K imaging experiment that does not experience a homogeneous ignition event. The pressure remains near-constant, as expected for CRV-fill experiments, and the OH emission rises over a long time interval of 3 ms (5-8 ms) as seems reasonable. However, the image data clearly shows that the ignition event is dominated by early burning in regions growing from the circumference, i.e. a non-uniform ignition event.



Figure 4. Multi-diagnostic study of non-uniform ignition. Reflected shock conditions: 986 K, 3.1 atm, n-heptane/21% O₂/argon, ϕ =0.5. Blue lines outline the side wall emission observation volume and the red line outlines the line-of-sight laser absorption measurement of fuel.

7 Conclusion

The ongoing improvement of shock tube performance will provide experimenters and modelers with higher quality measurements and lead to refinements in combustion kinetic models. These improvements have already led to reduced uncertainties in ignition delay time measurements because of stronger constraints on test gas temperatures and pressures, new studies of real fuels, such as diesel and jet fuels, and investigations at longer test times and lower temperatures, overlapping with rapid compression machine measurements. Imaging studies of measurements at longer test times in one of our shock tubes have revealed non-uniform ignition behavior in some experiments that calls into question the usual assumption of a homogeneous uniform reaction environment. A facility-dependent test-condition map is thus needed to identify the regimes where more detailed gasdynamic modeling is required for quantitative combustion kinetics experiments, and also to guide needed work on further facility improvements.

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