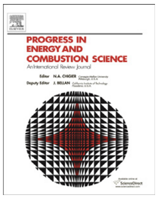
Progress in Energy and Combustion Science 44 (2014) 103–114

Contents lists available at ScienceDirect

Progress in Energy and Combustion Science

journal homepage: www.elsevier.com/locate/pecs



Review

Recent advances in laser absorption and shock tube methods for studies of combustion chemistry

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ARTICLE INFO

Article history:
Available online 5 June 2014

Keywords:
Shock tube
Laser absorption
Constrained reaction volume
Species time-histories
Isotopic labeling

ABSTRACT

Recent advances in laser absorption and shock tube methodologies for studies of combustion chemistry are reviewed. First the principles of shock tube operation are discussed, and then an overview of shock tube diagnostic methods and experiments is covered. Recent shock tube developments include the use of driver inserts to counteract the small pressure gradient seen in conventional reflected shock wave experiments and the use of a constrained-reaction-volume strategy to enable the implementation of near-constant-pressure gasdynamic test conditions during energetic processes. Recent laser absorption developments include the use of a CO_2 laser absorption sensor to accurately monitor temperature during shock wave experiments, the use of multi-wavelength laser absorption strategies to simultaneously monitor multiple species time-histories, and the used of isotopic labeling strategies to identify individual reaction sites during the measurement of elementary reaction rate constants. The improved ability to accurately constrain the test conditions in shock tube experiments, combined with non-intrusive, species-sensitive and quantitative laser absorption diagnostics, is enabling experimenters to provide a new generation of high-quality experimental kinetics targets for combustion chemistry model validation and refinement. The paper concludes with a brief discussion of newly emerging laser-diagnostic techniques and a summary of future research directions.

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http://dx.doi.org/10.1016/j.pecs.2014.05.001

1. Introduction

There is a growing role for shock tubes in studies of combustion chemistry, enabled particularly by the addition of laser-based species diagnostics and recent work to improve shock tube performance. In particular, the availability of solid-state tunable lasers developed originally for the telecommunications industry has recently opened up the infrared spectrum to laser absorption diagnostics and allowed sensitive access to many new species. As well, recently-implemented improvements in the operation of shock tubes now can provide near-constant-volume gasdynamic conditions (for low energy release processes) or near-constant-pressure gasdynamic conditions (particularly useful for large energy release processes). Both strategies allow the combustion modeler to implement high-fidelity modeling of the reactive gasdynamics processes as part of their analysis of reflected shock wave experiments. The improved ability to accurately constrain the test gas conditions in these ways, combined with non-intrusive, species-sensitive and quantitative laser absorption diagnostics, is enabling experimenters to provide higher-quality experimental kinetics targets for combustion chemistry model validation and refinement. In this paper we will overview recent advances in shock tube and laser methodologies for chemical kinetics.

1.1. *Principles of shock tube operation*

A shock tube is its simplest form is a long tube with closed ends separated into two sections by a diaphragm [1]. The test gas mixture is placed in the driven (low-pressure) end of the tube and the driver end of the tube is over-pressured with gas, often helium or a helium mixture, until the diaphragm bursts. A shock wave quickly forms and moves rapidly ahead of the driver gas expanding into the driven section. Conservation of mass, momentum and energy relations, along with the equation of state of the test gas and the measured speed of the shock wave, enable calculation of the step change in temperature and pressure of the moving test gas behind the wave. Upon reflection of this incident shock wave from the closed end wall of the driven section, the test gas is further compressed and heated to its initial pre-reaction temperature and pressure, and is effectively stagnated. Because of the near-one-dimensionality of the shock tube flow and the near-planar nature of the shock wave it is possible with a precise measurement of the incident shock speed to accurately determine (with $<\pm1\%$ uncertainty) the temperature and pressure behind the reflected shock [2]. Because of the effective step change in shock conditions and the effective stagnation of the test gas mixture behind the reflected shock wave, the test gas mixture can potentially be treated as a zero-dimensional reactor (excluding a very thin boundary layer) and modeled using either a constant-volume or constant-pressure constraint. However, important deviations from the idealized constraints are often present unless proper attention is given to experimental design.

One operational drawback of shock tube operation is the single-shot nature of the facility. This disadvantage can be avoided by the use of diaphragmless shock tubes. Recently, Tranter et al. have replaced the traditional diaphragm with a fast-acting valve [3]. This method has allowed repeated shocks at near-similar conditions and for certain diagnostics systems (e.g. time-of-flight/mass-spectrometry (TOF/MS)) has significantly improved the quality of measurements.

Tranter and Lynch also have extended this concept to a miniature high-repetition-rate shock tube [4]. This facility provides excellent reproducibility of high-pressure, high-temperature reflected shock conditions that enable the pioneering use of diagnostics based on synchrotron light sources, where many experiments need to be averaged to obtain adequate signal-to-noise levels. Using this facility, they have achieved repetition rates of 4 Hz, pressure up to 100 atm and reflected shock test times of the order of 100 μs [4]. Similar repetition rates in a small diameter (2 mm) diaphragmless shock tube have been achieved by Shiozaki et al. [5].

Experimental work with fast-acting valves has also been applied in larger shock tube facilities. Recent work by Heufer et al. has achieved opening times of order 1 ms for these valves [6]. Such systems provide the opportunity for a significant reduction in shock tube impurity loading that can occur with the pyrolysis of burst diaphragm particles.

1.2. *Capabilities of shock tubes*

A wide range of test gas conditions can be achieved in shock tubes. Typical reflected shock conditions for combustion chemistry studies cover temperatures from 600 to 3000 K and, depending on the construction and wall thickness of the shock tube, can cover pressures from sub-atmospheric to as high as 1000 atm as demonstrated by Tranter and co-workers [7].

Different configurations of shock tubes can be used for specific purposes. Large diameter shock tubes, typically 10 cm inside diameter and above, generally exhibit relatively small influences of boundary layers and provide test conditions that are closely predicted by the shock jump equations. Small diameter shock tubes (e.g. 5 cm diameter or less), however, can have boundary layers that are a significant fraction of the internal tube diameter, in which case the one-dimensional shock equations provide less accurate determinations of the test gas conditions; a discussion of this can be found in Michael and Sutherland [8]. Although kinetics studies can be conducted behind incident shock waves, most current work is performed using reflected shock waves.

Variations in the lengths of the two sections, driver and driven, can be used to vary the test time, defined as the time available when test conditions are approximately uniform. In a conventional shock tube, with a 15 cm internal diameter and a driven L/D of 70–100 and a driver L/D of 20–50, reflected shock wave experiments with nitrogen or argon as the carrier gas and helium as the driver gas have usable test times of 1–3 ms, often limited by non-ideal wave processes that occur when the reflected shock wave meets the moving driver gas-driven gas interface. Proper selection of driver gas composition, known as tailoring, can be used to obviate these non-ideal processes and thereby extend the reflected-shock test times to about 10 ms. Petersen and co-workers have explored the use of different driver gases that satisfy the tailoring condition while reducing the sound speed and thereby delaying the ultimate end of test time due to the arrival of the rarefraction wave of driver gases [9]. Using tailored driver gas mixtures of carbon dioxide–helium and/or propane–helium, they were able to achieve test times of 15 ms for a driver of length 3.5 m and a driven section of length 10.7 m at a reflected shock temperature of 891 K.

Figs. 1 and 2 are X–t diagrams that show the idealized wave structure during shock wave experiments. In Fig. 1 the test time is determined as the time between the arrival of the reflected shock wave at the test location and the arrival of the weak wave produced by the interaction of the reflected shock wave and the driven gas–driver gas interface. In Fig. 2 the test time is terminated when an expansion wave finally reaches the measurement location.

To investigate low-temperature regimes of combustion reactions, longer test times are generally required. This is of particular importance in studies of the negative-temperature-coefficient (NTC) ignition regime seen in diesel and other practical engine fuels. To extend the test time in a shock tube, two requirements are thus generally needed: a longer driver section to delay the return of