A high-pressure shock tube characterization and auto-ignition delay investigations

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Abstract

A high pressure shock tube “HPST” has been designed for the purpose of chemical kinetics studies at elevated pressures and temperatures. The present HPST is designed as a versatile tool and includes the features of a fast compression, optical accessibility, and capability for specie measurement. Characterization experiments establish the suitability of the tube for chemical kinetic studies and show that highly repeatable experimental conditions up to 40 bar and temperatures between 1300 and 2000 K can be obtained. As well, tailoring gas mixture in the driver section, used to obtain a longer test time, is studied in the characterization experiments. Using this facility, auto-ignition investigations are conducted for methane mixture (1% CH_4 ; 4% O_2 ; 95% Ar ; f=0,5) at 10, 20 and 40 bar pressures and temperatures from 1300 K up to 2000 K.

Introduction

A shock tube is an ideal reactor for studying chemical kinetics (auto-ignition characteristics of gas mixtures, flame velocity...) due to its gas-dynamic simplicity. Shock tubes create a high-temperature and high-pressure environment that ideally exhibits homogeneous, adiabatic, constant-volume (CV), stagnant gas conditions for the reacting mixture. Therefore, since virtually all non-kinetic processes such as fluid flow, heat transfer, transport, and turbulence are negligible, a shock tube can be modelled as a simple homogeneous, CV, adiabatic reactor. In a shock tube, an inert driver gas at high pressure is separated by a thin diaphragm from a several meter long section containing the potential reactants. Reactants are usually diluted in inert gas and prepared at significantly lower pressure. Puncturing the diaphragm creates a shock wave which compresses the mixture of reactants to a desired temperature and pressure. Usually ignition delay time is measured behind the reflected shock waves. Ignition delay time is defined as the time interval between shock arrival, which is determined from a pressure trace, and the onset of combustion, which is usually inferred from either a pressure trace and/or the emission/absorption spectra of an intermediate combustion species (e.g., CH*, OH*). In shock tubes, pressure and temperature up to 550 bar and 2800 K have been obtained [1]. However, the observation times are typically in the order of 1 ms.

According to literature, long test time, important to study combustion chemistry at low temperature in a shock tube, can be achieved by several methods. Davidson and Hanson [2] proposed two solutions to improve the performance of shock tubes. Non-ideal facility effect (manifested by incident shock attenuation and boundary layer) can engender a gradual variation in pressure (accompanied by a change in temperature) which is seen to rise about of 3 % per ms in non reacting region. This non ideal pressure rise influences the ignition time. The authors proposed a first solution to improve shock tube performance to provide uniform pressure and temperature by the addition of driver-section inserts. According to Davidson and Hanson, the first study which proposed to modify 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 was given by Dumitrescu [3]. A second solution is proposed by the authors, which can be added to the first one, by the use of a tailored gas mixture in the driver section. Helium is typically used as the driver gas since it has a high sound velocity as a result of its very low molecular weight [4] producing strong shocks.

However, high sound velocity reduces test times due to fast propagating expansion waves. Sound speed could be reduced by mixing He with heavier gases and/or having smaller specific heat ratios. Using a tailored gas mixture introduces a related uniformity issue which can cause a transient increase of pressure in the reflected shock pressure. The contact surface can be protected by introducing a short region of buffer gas volumes in the driven section immediately in front of the diaphragm. Same gases mixture as the driver is used as a buffer gas. The combination of tailored gas mixture, driver inserts and buffer gas enable a long test times of 8 ms with less than ± 3 % per millisecond of pressure fluctuations [5].

When facility modification is not an option, using a tailored gas mixture in the driver section can be used; tailoring with He/Ar or He/N_2 mixtures may not work if the driver section is too short against the driven one [5]. Amadio et al. [5] used He/CO_2 and He/C_3H_8 mixtures in their experiments leading to a test time up to

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14.5 ms. Therefore experimental conditions (Initial pressures (P_1 and P_4), driver gas composition, driven gas used) are studied in this work to characterize the shock tube which can lead to a better understanding how to have a longer test time. Longer test times were achieved in this study to create a junction between auto ignition delay measurements using HPST and other facilities like rapid compression machine (RCM).

Auto-ignition delay was measured in this work for Methane-Oxygen-Argon mixtures, compared with previous studies [6] and with prediction based on NUI Galway mechanism [7].

Apparatus

The experiments were carried out in a high-pressure shock tube with an internal diameter of 50 mm. The tube is divided by a double membrane (Mylar diaphragm) into two sections; a driver section of 4 m and a driven section of 5 m, constituting a small section called "intermediate section (IS)". The end-wall flange can be removed for cleaning purposes where Ethanol is used for cleaning the driven section. In addition of the main tube, this facility includes a vacuum system, a velocity detection system, an optical detection system and a data acquisition system. Light emission from OH* chemiluminescence can be collected through a quartz window located at the sidewall. A narrow pass band filter and a high voltage photomultiplier are used for this emission detection where signal is recorded using a National Instrument Compact RIO with a frequency of 1 MHz and transferred to a computer for signal processing. A schematic of the shock tube and its gas-handling system can be found in Fig. 1.

The whole tube was pumped down to pressures below 5 Pa using a roughing pump (PFEIFFER Vacuum). Note that in this specific study, the need for ultra-low vacuums is reduced by the fact that high-pressure gases are used to fill the tube to its initial condition, so the relative impurities are smaller. The vacuum pressure is controlled using a PFEIFFER pressure gauge. The absolute filling pressures in "driven section" and "intermediate and driver sections" are measured using two Kistler pressure transducers (4260A / 4262A) with ranges 0-5 bar and 0-50 bar respectively.

Under normal circumstances, the shock tube is pressure-driven using helium as the driver gas. However, driver-gas tailoring was used to obtain longer test times. This is discussed in more detail in the next section. For experiments at room temperature, Mylar diaphragms of thickness ranging from 100-350 µm are used. Puncturing of those diaphragms, creating the shock wave, is obtained by using a vacuum reserve leading to an instant pressure decrease in the IS section.

Post-shock pressures are measured using a Kistler piezoelectric pressure transducer (603B) in combination with an amplifier. This Kistler pressure transducer is located at the bottom of the tube, 30 mm from the end-wall. This transducer is used to determine the qualitative, transient pressure and to ascertain the timing of the experiment. Absolute pressure readings are not obtained from this Kistler pressure transducer but instead are calculated using the shock speed in conjunction with the 1-D shock relations, the species thermodynamics and the initial filling pressure (Kistler 4260A).

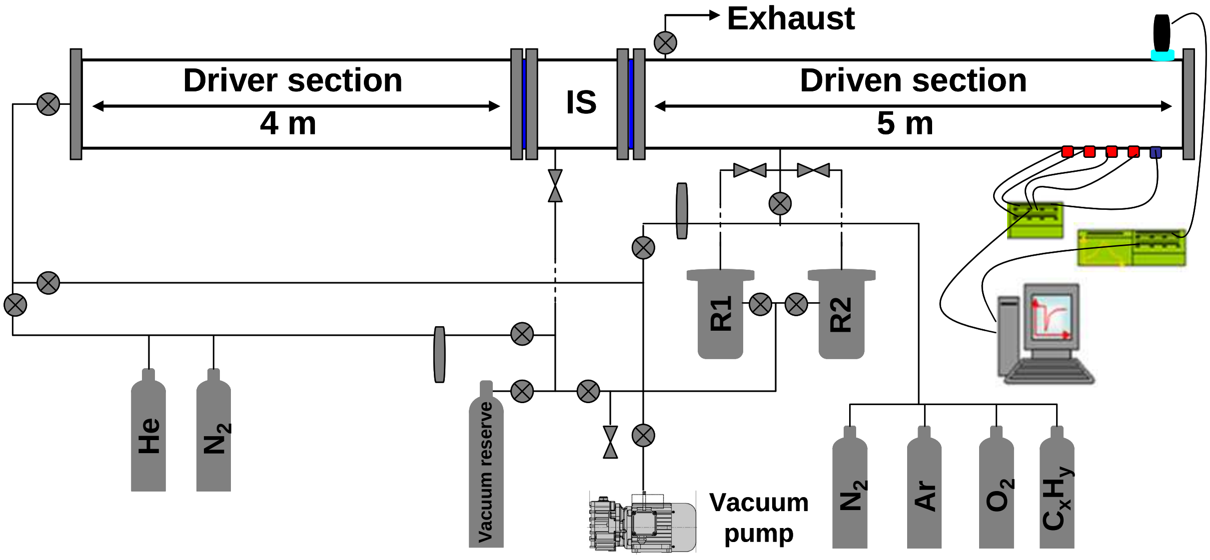

Figure 1: Sketch of the experimental apparatus

In all experiments, the shock wave velocity had to be calculated as accurately as possible. This is because the wave speed, in addition to the familiar gas dynamic equations for normal shocks, is used to obtain the temperature. In fact, the conditions behind the reflected shock wave depend only on the speed of the incident wave, the initial fill pressure conditions, and the known gas properties. The normal shock assumption is specifically valid after a length of a few diameters away from the diagram. Non-ideal effects such as viscosity, imperfect diagram rupture and shock acceleration due to energy release in the reacting mixture can contribute to an axially non-uniform shock speed. To compensate for this natural attenuation of the shock, 4 individual piezoelectric pressure transducers (PCB 113B22) plus the Kistler piezoelectric pressure transducer (603B), with a time response less then 1 µs were used for the velocity measurements, providing 4 axial (and hence time) intervals. Based on these values, the incident shock wave velocity is extrapolated at the end wall. A mixing tank can also be used for fuel mixture which can be heated and magnetically stirred. For experiments in this study gases are directly introduced in the tube.

Characterization

The characterization of the shock tube is used to determine the initial experimental conditions (pressures in the driver and driven sections, nature of the carrier gas and diluents used ...) that will be used to carry out the fuel mixture experiments at a pressure and temperature well defined. In this section, reproducibility of experiments in non reacting gas (Argon) and tailoring gas mixture in driver section is also studied. As the shock tube used herein has a fixed geometry wherein the driver and the driven section have almost same length (4 against 5 m), longer test time were obtained only with tailoring gas mixture. Therefore, in the aim of this work, four conditions have been put in place and in order to have a pressure behind the reflected shock wave of 10, 20 and 40 bar: He/Ar, He(75%)-N_2(25%)/Ar, He(50%)-N_2(50%)/Ar and He/N_2.

As previously mentioned, usually, shock tube test times are on the order on 1 ms. To study combustion chemistry at low-to-intermediate temperatures, it is of great importance to increase the shock-tube test times. This can be done by tailoring the interface between the driver and driven gases. The shock-tube test time is defined as the time between the passing of the reflected shock wave and the arrival of the next wave, usually the expansion wave coming from the driver section. As said, strong incident shock waves are desired for high test temperatures (T_5), therefore helium is usually the gas of choice for the driver gas.

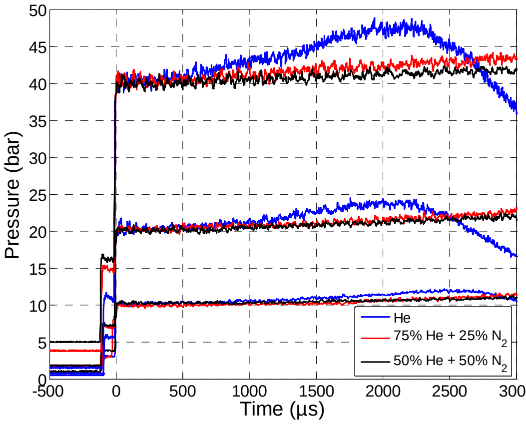

Figure 2: Impact of gas tailoring on the reflected pressure profile

The initial conditions studied are the pressure P1 (pressure of the diluents gas in the combustion section) and the pressure P4 (the carrier gas pressure in the motor section) at atmospheric temperature. Then the velocity of the reflected shock wave "Vref" is experimentally calculated from the measurements obtained by the pressure transducers and the piezoelectric sensor Kistler. Pressure "P5" and temperature "T5" behind the reflected shock wave are calculated using the chemical equilibrium software "Gazeq"[8]. The test time is finally determined for each condition at the pressures 10, 20 and 40 bar. It can be seen from figure 2, that gas tailoring as a positive impact on the pressure profile and results in a longer duration at constant pressure. However, results show that using 50% nitrogen in the driver gas is enough to increase the test time up to 3 ms.

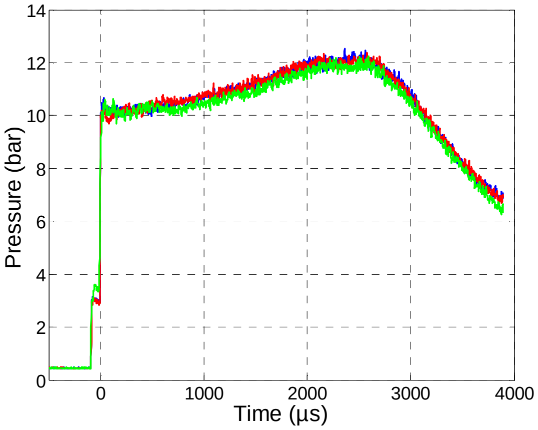

Figure-3: Comparison for three pressure profiles obtained for: He / Ar at P_5 = 20 bar

All initial conditions and results obtained for each pressure behind reflected shock are summarised in the table below (table 1).

All values shown in the table represent the mean values obtained and a maximum of error estimated on the temperature T5 is about 40 K for 1000K. The characterization of the shock tube is important to understand the limits of our facility and to verify the reproducibility of measurements obtained by this device. Test time can be increased by a factor up to 2.7 when using tailored gas mixtures in the driver. This increase in test time offers a reliable measurement of auto-ignition delay by shock tube facility; which will be used to clarify the junction between MCR and shock tube auto-ignition delay measurements. A very good reproducibility of all experiments is obtained for the three pressures studied. An example of comparison for three experiments at the same condition is presented in the figure 3.

Validation

This high pressure shock tube is validated by comparing auto ignition delay measurements obtained in this study with those given by Zhang et al. [6] at 10 and 20 bar and with prediction based on the latest NUI Galway mechanism [7]. Experiments achieved in this study were obtained using a premixed methane mixtures (1% CH_4; 4% O_2; 95% Ar ; • =0,5), delivered and calibrated by Air Liquid; those gases are directly introduced in the driven section of the tube. A very good agreement is obtained between experimental results obtained in this study with those obtained by Zhang et al. [6] for both pressures 10 and 20 bar. A comparison is shown in the Figure-3 below

Tailored gas mixtures were used only for experiments with an auto-ignition delay over 1 ms to ensure a variation of a pressure increase lower than 3% per millisecond before auto-ignition. Compared with calculated values obtained using the NUI Galway mechanism [7], a satisfied agreement is obtained validating a dependence of auto-ignition delay with temperature and pressure. Auto-ignition delay decrease with increasing temperature and pressure due of an increase of the activation energy affecting intermediate reaction which effectively promotes ignition. The comparison between experimental values and the ones calculated is shown also in Figure-3.

For P5= 10 bar

	P1	P4	P5	$V_{réf}$ (m/s)	T5	Test time (µs)
He/Ar	0.45	10.8	10.2	734	1298	1000
He(75%)-N_2(25%)/Ar	0.7	14	10	631	989	1600
He(50%)-N_2(50%)/Ar	1	16	10.5	574	837	2400
He/N_2	0.5	11	10.5	776	839	1300

For P5= 20 bar

	P1	P4	P5	$V_{réf}$ (m/s)	T5	Test time (µs)
He/Ar	0.7	22	20.2	798	1512	1000
He(75%)-N_2(25%)/Ar	1.6	26	20.2	607	924	1700
He(50%)-N_2(50%)/Ar	1.8	30	20	584	863	2000
He/N_2	0.7	22	19.5	850	955	1000

For P5= 40 bar

	P1	P4	P5	$V_{réf}$ (m/s)	T5	Test time (µs)
He/Ar	1.5	42	40.3	778	1444	700
He(50%)-N_2(50%)/Ar	3.8	48	40.2	575	840	2400
He(50%)-N_2(50%)/Ar	5	50	39.8	529	725	2700
He/N_2	1.7	43	40.3	807	886	1400

Table. 1: Initial conditions and the results obtained

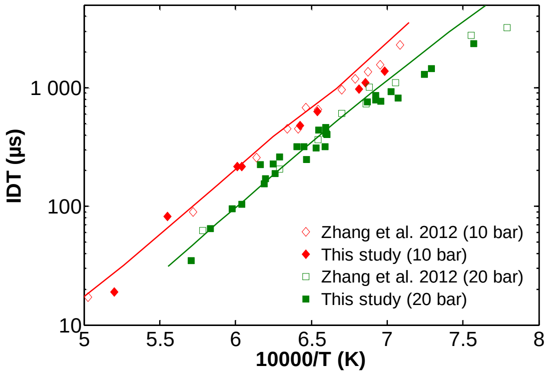

Figure-3: Comparison of results obtained in this study with those obtained by Zhang et al. [6] and with the NUI Galaway mechanism [7]

Auto-ignition delay was also measured for the same mixture at 40 bar which was well predicted by the NUI Galway mechanism (Figure-4) ; demonstrating the ability of the shock tube for experimental studies at elevated pressures.

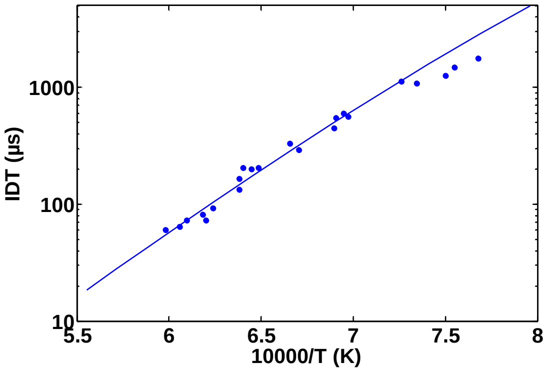

Figure-4: Comparison of results obtained in this study at 40 bar with the NUI Galaway mechanism (Metcalfe et al. 2013)

Conclusions

In summary, a high pressure shock tube was validated for auto-ignition delay measurements up to 40 bar and for a temperature range from 1300 up to 2000 K. Experimental results obtained herein were in a good agreement with previous experimental studies. As well, The NUI Galway mechanism reproduced satisfactory our experimental values obtained for a Methane mixture (ϕ= 0,5) highly diluted with Argon at 10, 20 and 40 bar after reflected shock wave. A tailored driver gas mixture must be used for auto-ignition delay measurements at low to intermediate temperatures (800-1300 K), where the delay is longer than 1 ms. The tailored surface ensures a minimum variation of pressure after reflective shock wave. Those experiments at long auto-ignition delay are important to check the ambiguity between the two facilities Shock tube and Rapid compression machine in future work. In further studies, this shock tube will be used for characterization of standard and bio-fuels.

Acknowledgments

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