On the Dynamics of Ignition Process behind Reflected Shock Waves under the Influence of Bifurcation

Owen Pryor, Samuel Barak, Erik Ninnemann, and Subith Vasu
Center for Advanced Turbomachinery and Energy Research (CATER),
Mechanical and Aerospace Engineering,
University of Central Florida
Orlando, FL 32816, USA

1 Introduction

Shock tubes are typically used to measure ignition delay times - a fundamental property of fuels that is a function of temperature, pressure, and mixture concentrations. Bifurcation is the separation of the normal reflected shock wave splitting inside the boundary layer to form to opposing oblique waves. Bifurcation occurs because the boundary layer that is formed behind the incident shock wave is not able to negotiate the pressure rise across the reflected shock, and is therefore trapped and carried along at the base of the shock near the sidewall [1, 2]. Bifurcation features normally appear in diatomic and polyatomic gases (such as fuel/air mixtures, mixtures with CO_2) but not in argon diluted mixtures and its features have been well-known through experimental visualization utilizing color schlieren [3] and side-wall pressure measurements [4, 5]. Bifurcation has been modeled in many computational studies [6-9]. Bifurcation affects determination of time zero because of the uncertainty in determining the arrival of the normal shock wave at the sidewall location and its effects are severe as one moves away from the endwall and also for short ignition delay times (<100 μs). In addition, it is commonly assumed that bifurcation should not affect the core portion of the post-shock region, which comprises most of the flow area [4]. However, a comprehensive study using multiple diagnostics to verify the influence of bifurcation and inhomogeneity on chemical kinetics is lacking in the literature though similar studies in rapid compression machines[10] have been carried out. In this work we focus on studying $CH_4/H_2/CO$ ignition in O_2 under the influence of bifurcation in heavily CO_2 diluted mixtures. Multiple diagnostic techniques are used to determine accurate ignition delay times when bifurcation is present.

2 Experimental Procedure

All of the experiments of this study were taken with a stainless steel shock tube. This shock tube has an inner diameter of 14.17 cm. The driver side is filled with helium and separated by a polycarbonate Lexan diaphragm. The driven side is filled to a specified pressure with a mixture prepared in a separate tank.

Correspondence to: subith@ucf.edu

When this diaphragm ruptures, a shock wave is formed and quickly travels down the driven side of the shock tube and heats up the test mixture. Five piezoelectric pressure transducers (PCB 113B26) placed along the last 1.4 m of the shock tube were used to measure the incident shock wave velocity using four time-interval counters (Agilent 53220A). The incident shock wave attenuation was always less than 2%. With the known velocity and a measured initial temperature and pressure of the driven side, one dimensional ideal shock relations can be used to calculate the reflected shock wave temperatures and pressures [11].

Mixtures were created using a separate 33 L mixing tank attached with to the shock tube through a gas manifold. Mixtures were prepared using the partial pressure method using two MKS baratrons with full scale ranges of 100 and 10,000 torr, respectively. For all experiments, lab grade gases from NextAir with purities of 99% or higher were used.

Data was recorded using a NI PCI-6133 Data Acquisition Device at 2MHz per channel. Measurements were taken radially at a test section 2 cm from the driven side end wall that contains eight ports. One of the ports has a piezoelectric pressure transducer (Kistler 603B1) to measure the pressure in the driven section. Another port contained a GaP transimpedance amplified detector (Thorlabs PDA25K) operating in the wavelength range between 150 and 550 nm. This detector is used to measure the emissions of combustion. No filters were placed in front of this detector in order to receive a clean signal from the experiment. A distributed-feedback inter-band cascade laser centered at a wavelength of 3.4034 μm (Nanoplus DFB ICL) detailed in [12-15] was used only to determine time-zero by the laser schlieren spike of the arrival of the reflected shock wave at the measurement location.

The ignition delay time measurement was defined as the time interval between the arrival of the reflected shockwave and the onset of ignition at the measurement location. The arrival, or time zero, was determined by the laser schlieren spike of the laser. The onset of ignition was determined by evaluating the time history of the emissions and finding the steepest rise and then extrapolating down to the baseline measurement (method A). This method was described in a previous study [16]. This ignition onset was compared with the high speed imaging of the combustion event. The measured ignition delays were also compared with the predictions of two reaction mechanisms (GRIMech 3.0 [17] and AramcoMech 2.0 [18]).

High speed imaging of the shock tube was taken using a Phantom V710 camera. The camera has a 1280x800 pixels CMOS sensor that is adjustable with the computer program Phantom Camera Control Application (PCC) to 256x256 pixel resolution at 67,065 frames per second. These settings enable a time resolution of 14.91 μs. The camera starts capturing images and is triggered by the output voltage of the Kistler type pressure transducer. Buffer images were taken before the triggering event as well. The camera is focused at the 2cm measurement location of the shock tube. A Fused Quartz end wall replaced the original stainless steel end wall to allow transparency. The images are post-processed on Matlab and the emissions are indexed in a matrix. Each element in the matrix is normalized to the highest intensity element (i.e. brightest image of the experiment). A false-color heat map is applied to each image with a circle drawn at the edge of the images to highlight the shock tube diameter. A camera emissions plot is then evaluated using the peak of the GaP transimpedance amplified detector and included in the plots of the data collection. The Color and Spectral Response Curve, [19], of the camera was then evaluated. Further details of this setup and details of the plot being normalized to the emissions detector can be found in [20].

3 Results and Discussion

To understand the effects of bifurcation on the dynamics of shock tube experiments, two different fuels were studied. The first fuel was mixtures of methane with various levels of CO_2 as the diluent. The experiments were studied for an equivalence ratio of 1 at around 1 atm. The carbon dioxide dilution ranged from 0% to 89.5%. The temperature range for the methane experiments ranged from 1600 to 2000 K. The second fuel that was studied was various combinations of syngas. Syngas is a combination of hydrogen and carbon monoxide that is created from the gasification of coal. The temperature range for these experiments ranged from 1000 to 1300 K. The equivalence ratio was varied between $\phi = 0.5$ to 1.0.

Figure 1 displays images of the ignition process for the mixture without bifurcation (X_{CH4}=3.5%, X_{O2}=7%, X_{Ar}=89.5%). For the imaging of this mixture, it can be seen that most of the experiments start around where the window plugs sit before rapidly combusting homogeneously. It can also be noted that the flame fills the entire cross-section of the shock tube by the location of peak sidewall emissions with small voids located around a circle just inside of the wall. By comparing different experiments at the same time at the same points of ignition, several interesting similarities are capable of being drawn. First each of the images show that the flame takes approximately the same amount of time to propagate from the top left corner to the rest of the shock tube, occurring in approximately 75 μs from the first image when there is very little emission from combustion. It can also be noted that although each of the runs have small voids around the edge of the flame, each of the voids had been part of the flame at some point in the combustion process. At the conditions present for this mixture, it is clear that the flame propagates throughout the entire shock tube cross-sectional area and remains there until the arrival of the reflected expansion waves.

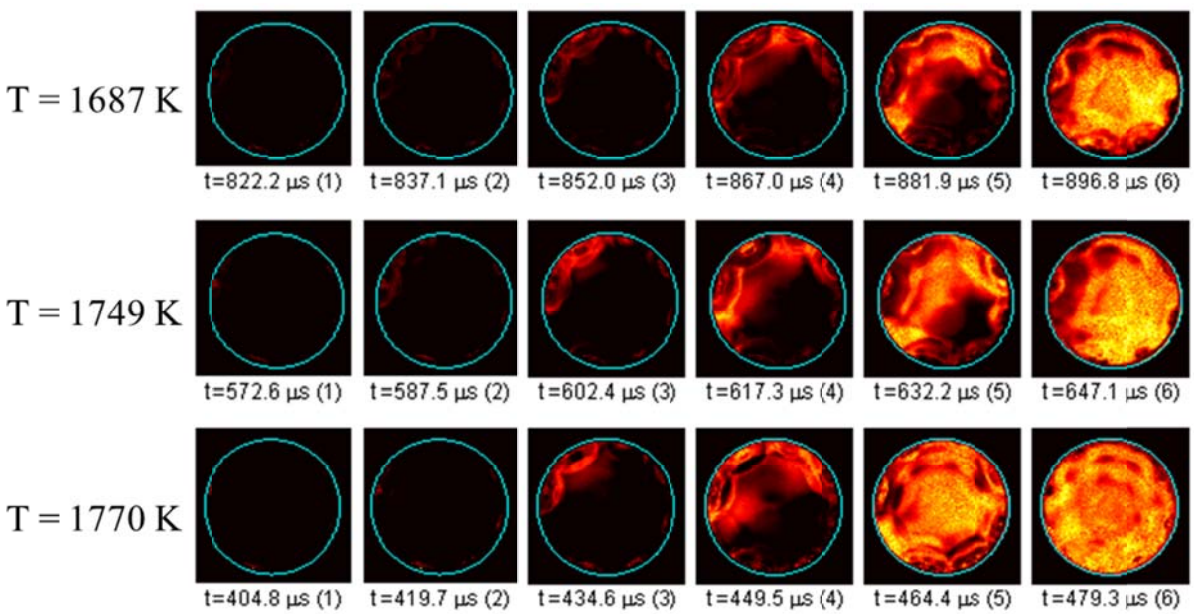

Figure 1. Comparison of high speed camera images for different temperatures mixture without bifurcation (X_{CH4}=3.5%, X_{O2}=7%, X_{Ar}=89.5%). All intensities were normalized to the highest pixel intensity of the last image for each individual run.

Bifurcation had a dramatic effect on all of the diagnostics as expected. Provided in Fig. 2 are the images of the ignition process at three temperatures for mixture with bifurcation (X_{CH4}=3.5%, X_{O2}=7%, X_{Ar}=29.5%, X_{CO2}=60%). By comparing the very last images (i.e. sixth image) taken at each temperature, one can realize the decrease of the flame area ratio as the temperature is reduced. The flame area ratio (the ratio of the visible emission to the cross-sectional area) increases from 0.288 at 1724 K to 0.452 at 1951 K. The reason for this trend can be explained by the fact that bifurcation occurs when the boundary layer does not have sufficient momentum to pass through the normal shock wave. Therefore, anything decreasing the momentum such as the decrease of temperature or specific heat ratio (speed of sound is given by $a = \sqrt{\gamma RT}$) would escalate the severity of bifurcation. For example, increasing CO_2 percentage in the mixture from 60 to 85% causes the flame area ratio to decrease from 0.806 to 0.452 around 1900 K. This trend happens for the same reason. In other words, the mixture specific heat ratio decreases when XCO_2 is increased, because $\gamma_{CO2} = 1.28$, whereas $\gamma_{Ar} = 1.66$.

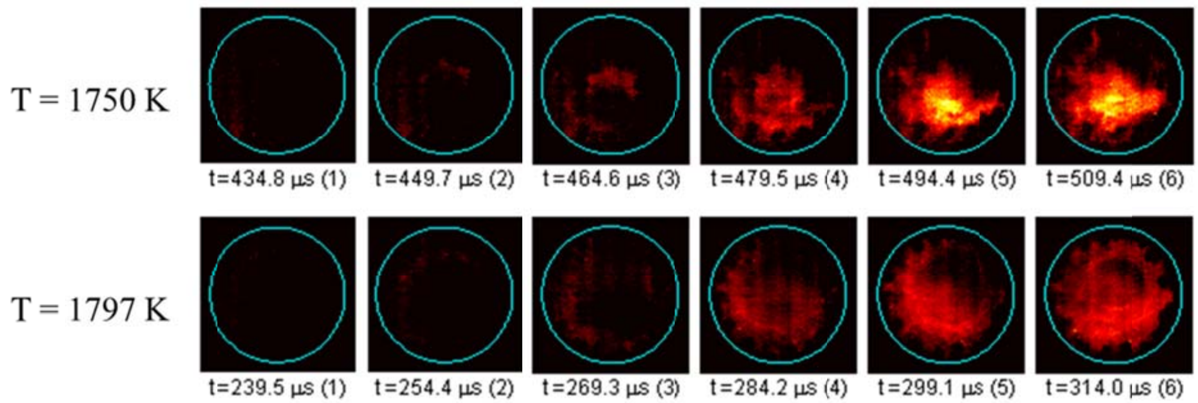

Figure 2. Comparison of high speed camera images for different temperatures of mixture 2. All intensities were normalized to the highest pixel intensity of the last image for each individual run.

Figure 3 is a pressure trace of 5% H_2 + 5% CO + 10% O_2+ 20% Ar+ 60% CO_2 experiment with bifurcaiton. Measurements were conducted in various fuel concentrations (H_2/CO ratios, Θ) and bifurcation levels (X_{CO2}=0-90%) at an equivalence ratio (Φ) = 1. Bifurcation is clearly visible during the rise associated with reflected shock waves. A clear pressure rise is seen in the experiment that matches the emissions detector. The high speed camera was able to capture the ignition event as well. The end wall emissions from the camera are lagged compared to the sidewall emissions detector, however, it eventually observes more light than the detector as evident of the steeper rise of the slope compared to the camera emissions. Figure 4 shows end wall images of the flame at the time defined using the slope method (A) and at the peak of emissions (B). It is clear that the slope method is an accurate representation of the time when homogeneous ignition takes place inside the shock tube. The data points collected using the slope method are compared with the predictions of two combustion chemical kinetic mechanisms for syngas combustion (GRIMech 3.0 [17] and AramcoMech 2.0 [18]) and shown in Figure 5. The simulations were conducted using the CHEMKIN PRO [21] and using constant-volume, internal energy (constant V, U) assumption. Both mechanisms are able to predict the trend seen in experiments as a function of temperature. However, there is slight disagreement in magnitude between measurements and predictions, which will be investigated in detail in the future.

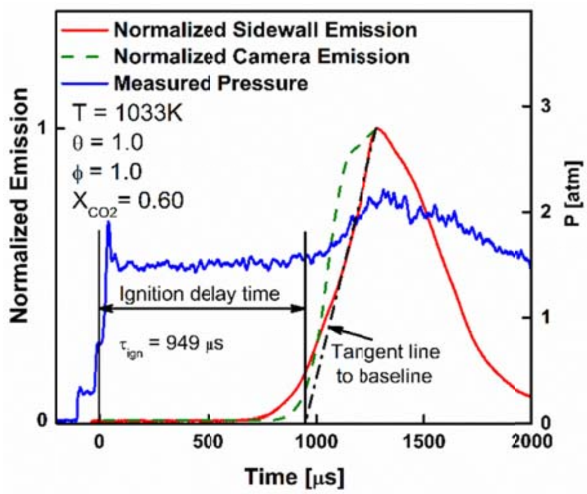

Figure 3. Sample Experimental Pressure Trace. Mixture is 5% H_2 + 5% CO + 10% O_2+ 20% Ar+ 60% CO_2

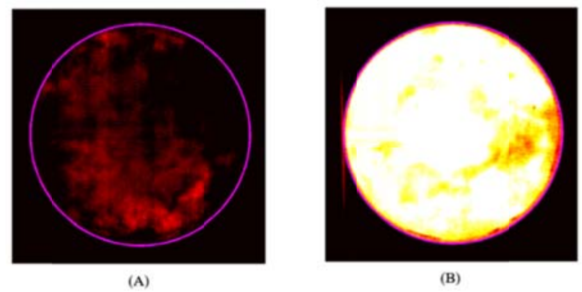

Figure 4. Sample endwall imaging data for experiments presented in Figure 3. Endwall images of ignition at the ignition time definition according to (A) the slope method and (B) at the peak of emissions.

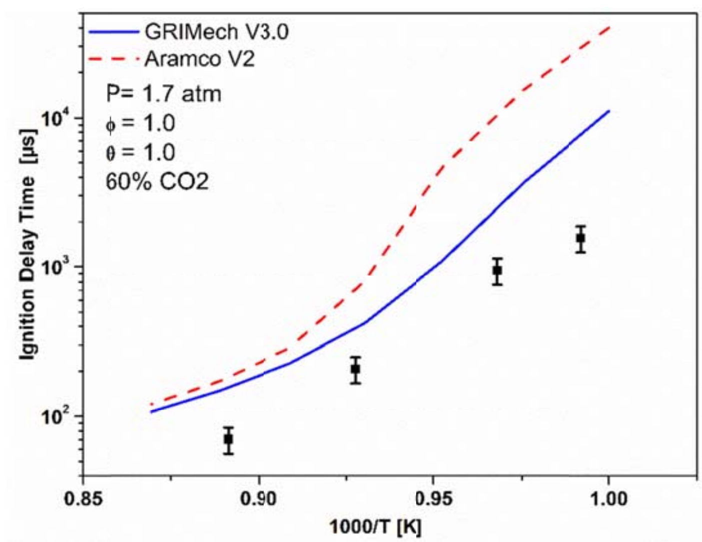

Figure 5. Comparison of experimental and predicted (GRIMech 3.0 [17] and AramcoMech 2.0 [18]) ignition delay times. Mixture is 5% H2 + 5% CO + 10% O2+ 20% Ar+ 60% CO2.

4 Summary

Ignition delay times from shock tubes are a common method to look at the global reactivity and to validate combustion chemical kinetic mechanisms. Traditionally, shock tube experiments are carried out with argon as a diluent when shock tube behaves ideally. With the addition of CO_2, there is much more uncertainty in the ignition delay time measurement due to a reduction in the emissions signal caused by bifurcation, which is a fluid effect that causes concerns for perceived 0-D shock tube experiments. In order to understand the dynamics of the shock wave ignition, high speed camera images were taken for two different fuels, methane and syngas, to understand the effect of CO_2 and bifurcation on the combustion process. It has been shown that the ignition delay time measurements were able to be captured with CO_2 dilution but the actual ignition process is not homogeneous based on the imaging. The images showed that the ignition event was confined to a much smaller cross section than in an argon bath. The chemical kinetic mechanisms were unable to predict the ignition delay times. To better understand bifurcation and ignition phenomena, additional experiments in CO_2 dilution needs to be performed in the future.

5 References

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