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# **New experimental insights into acetylene oxidation through novel ignition delay times, laminar burning velocities and chemical kinetic modelling**

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<b>References</b>	<b>(35+2) * 2.3 * 7.6</b>	<b>646</b>
<b>Tables</b>	<b>[(6+2) * 7.6 * 2] + [(5+2) * 7.6 * 2]</b>	<b>228</b>
<b>Figures and captions</b>		<b>1385</b>
<b>Total</b>		<b>6174</b>

**Figures and captions:**

<b>Fig.</b>	<b>height(cm)</b>	<b>height(mm)</b>	<b>plus 10</b>	<b>*2.2</b>	<b>*columns</b>	<b>captions</b>	<b>Total</b>
1	5.06	50.6	60.6	133.32	133.32	21	155.3
2	5.05	50.5	60.5	133.1	266.2	12	278.2
3	5.04	50.4	60.4	132.88	132.88	21	153.8
4	7.6	76	86	189.2	189.2	33	222.2
5	5.05	50.5	60.5	133.1	133.1	13	146.1
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## Abstract

The oxidation of acetylene is central to the oxidation of virtually all hydrocarbon fuels. It is also important in the commercial industry, due to its wide range of applications such as, flame photometry, atomic absorption, welding etc. In *this study*, ignition delay times (IDTs) for acetylene oxidation were measured at elevated pressures (10–30 bar) and temperatures (700–1300 K) in a high-pressure shock-tube (HPST) and in a rapid compression machine (RCM). The range of pressures, temperatures and mixture compositions studied are at conditions never previously investigated in the literature. The new measurements highlight some major shortcomings in our understanding of the oxidation mechanism of acetylene. The importance of these findings is accentuated, considering the fundamental nature of acetylene chemistry in modelling larger hydrocarbons. These data are complemented by new laminar burning velocity (LBV) experiments, independently performed in two different laboratories. As commercial cylinders commonly contain acetylene gas dissolved in acetone, we have also tested the influence of acetone on acetylene reactivity. It was found that the measured LBVs in both laboratories decreased when acetylene dissolved in acetone was used versus when the pure acetylene was used. The IDTs displayed no such sensitivity. When compared to the literature data, the new LBVs for pure acetylene displayed a pronounced increase in the fuel-rich regime, and the peak flame speeds from TAMU and RWTH increased by about 21 and 14 cm/s, respectively. The kinetic models, with one exception, over-predict the measured IDTs by an order of magnitude at temperatures below ~1000 K. The reaction of acetylene with hydroperoxyl radicals is critical in accurately predicting the low-temperature, high-pressure IDT data. The experimental findings together with the interpreted models, highlight the need for further work to better understand acetylene oxidation.

**Key words:** Acetylene; ignition delay time; high pressure shock tube; rapid compression machine; constant volume vessel.

## 1. Introduction

Understanding, and accurately predicting, the oxidation of small gaseous compounds is essential in hierarchically developing accurate kinetic models of heavier hydrocarbons [1]. Acetylene ( $C_2H_2$ ) is one of the major intermediates produced in the oxidation of larger hydrocarbons and is a prominent precursor in soot formation, especially at fuel-rich conditions [2]. Previous  $C_2H_2$  oxidation studies were conducted in shock tubes (ST) [3-8], with species versus temperature/time studies performed in jet-stirred reactors (JSRs) [2, 9, 10] and LBVs also measured [11-16]. Most of the studies have focused on  $C_2H_2$  flames due to its very high flame temperature compared to other hydrocarbon fuels, since one of its main applications lies in welding and cutting [17].

$C_2H_2$  ST studies have focused on pyrolysis chemistry [6, 18-20] and despite its importance, oxidation studies have been limited to low pressures. Eiteneer et al. [3] reported IDT experiments by varying compositions of acetylene (i.e. 0.25, 0.50, 1.0%) and oxygen diluted in argon, at equivalence ratios ( $\phi$ ) of 0.06–1.66, at temperatures of 1150–2132 K and at pressures of 0.9–1.9 atm. Fournet and co-workers [4] studied acetylene oxidation at 1.0 and 3.0% acetylene at temperatures of 1000–1650 K and pressures in the range 8.5–10 bar. Gardiner et al. [5] used  $CH^*$  and  $OH^*$  emissions to measure IDTs, which were performed for various mixtures at 1.0% acetylene composition and temperatures of 1500–2500 K at pressures of 0.006 and 0.013 bar. Hidaka et al. [6] studied acetylene oxidation for various compositions of acetylene ranging from (0.5–4.0%) in the temperature range 1100–2000 K at pressures of 1.1–2.6 atm. Homer et al. [7] investigated 0.5% acetylene + 0.8%  $O_2$  diluted in Argon at temperatures of 1580–2300 K and at pressures of 0.6–0.7 bar. Jachimowski [8] used a ST to investigate acetylene ignition behind incident shock waves by measuring the radiation profiles from carbon monoxide and carbon dioxide using acetylene compositions of 1.0, 1.5, 1.94%, at temperatures in the range 1815–2365 K and at pressures of 1.1 and 1.7 atm.

Early modelling work by Varatharajan and Williams [21] predicted the presence of a negative pressure dependence for acetylene IDTs, using constant-volume predictions at the conditions of interest to *this study* (Fig. 1). Herein, we show that four widely used chemical kinetic models also predict an inverse pressure dependence for acetylene IDTs. However, there are no experimental data available to verify the predictions of this atypical ignition behaviour, which is only verified previously for H<sub>2</sub>/O<sub>2</sub> mixtures [22].

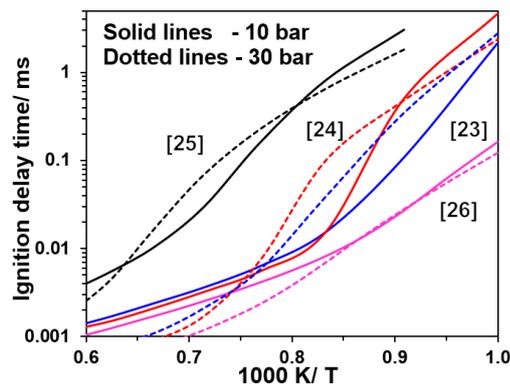


Fig. 1. Predictions of acetylene oxidation in air at  $\phi = 1.0$  using AramcoMech2.0 [23], San Diego Mechanism [24], GRI-Mech 3.0 [25], and Glarborg Mechanism [26].

Egolfopoulos et al. [13] studied LBVs of C<sub>2</sub> hydrocarbons at room temperature for fuel-lean to fuel-rich mixtures at pressures ranging from 0.25–3.0 atm, but acetylene was limited to pressures below 1 atm and diluted in air due to safety concerns. Jomass and co-workers [14] performed experiments for three C<sub>2</sub> and two C<sub>3</sub> hydrocarbons in air, at pressures of 1, 2 and 5 atm, at equivalence ratios of 0.6–2.0, but limited acetylene experiments to pressures below 2 atm. LBV data for C<sub>2</sub>H<sub>2</sub>/air mixtures at 1 atm and 298 K by Egolfopoulos et al. [13] and Jomass et al. [14] reasonably agree in the fuel-lean regime, while a pronounced divergence is seen in the fuel-rich regime (20% difference at  $\phi = 1.4$ ). Jomass et al. [14] stated the reason for over prediction of LBVs by Egolfopoulos et al. [13] is due to the linear extrapolation method employed for data extraction. The Park et al. [15] data for C<sub>2</sub>H<sub>2</sub>/(13%O<sub>2</sub>+87%N<sub>2</sub>) mixtures agree with those of Egolfopoulos et al. [13] at 1 atm and 298 K, although the LBV data extraction methods are different. Ravi et al. [11] concluded

that their LBV data for acetylene/air mixtures at 1 atm and at an unburnt temperature of 298 K agree with those of Jomass et al. [14]. Shen et al. [12] concluded that their data agrees within 10% of Jomass et al. [14] for C<sub>2</sub>H<sub>2</sub>/air at 1 atm and 298 K over the whole equivalence ratio range. Rokni et al. [16] investigated LBVs of various mixtures of acetylene in air over a wide range of equivalence ratios 0.6–2.0, at un-burnt gas temperatures of 300–590 K and at pressures from 0.5–3.3 atm. The experimental data consistency is highly important, as they are widely used to validate the predictions of kinetic models. Despite the wide range of literature data at the same conditions (1 atm and 298 K), there is still an outstanding question on the discrepancy of LBVs of acetylene for  $\phi > 1$ .

The aims of *this study* are three-fold, (i) to provide a new set of experimental IDT data for acetylene oxidation over a wide range of temperatures and equivalence ratios, at elevated pressures; (ii) to provide reliable LBV data for acetylene/air at 1 and 2 atm and 298 K; and, (iii) to interpret the experimental results with available chemical kinetic models from the literature. By doing so, we have found that only the Glarborg mechanism [26] is able to reproduce the newly measured IDT data with any reasonable degree of accuracy. The main reason for this is different models' treatment of the reaction of acetylene and hydroperoxyl radical, as will be explained in detail later. Furthermore, the effect of acetone, in which acetylene is commonly dissolved, is considered and found to measurably influence LBVs, resulting in decreased laminar burning velocities. This decrease in the LBVs is found to align with a number of literature measurements. However, when LBVs of pure acetylene are measured in two independent laboratories, the measurements are faster relative to the reported literature. Hence, experiments were performed to help unravel these discrepancies.

## 2. Experimental Methods

Two independent facilities have been used to measure IDTs of acetylene at pressures of 10, 20 and 30 bar and at  $\varphi = 0.5, 1.0$  and 2.0. Faster IDTs (0.02–2.0 ms) were measured in the HPST at NUIG and relatively slower IDTs (3–100 ms) are measured in the RCM at PCFC, RWTH Aachen University. These facilities complement each other, covering a relatively wide temperature range. The experiments performed in these two facilities are listed in Table 1. A new set of LBVs was measured in a constant-volume vessel at TAMU at 1 and 2 atm and 298 K for  $\varphi = 0.6$ –2.0. These data are complemented by the LBV experiments performed in a spherical combustion chamber at ITV, RWTH Aachen University.

### 2.1 High pressure shock tube (NUIG)

The NUIG HPST was described previously [27] and is only briefly discussed here. The 9 m long stainless-steel tube with uniform cross-section of 63.5 mm inner diameter is divided into three sections; a driver (3 m), driven (5.7 m) and double-diaphragm section (30 mm). The double-diaphragm section, with inserted pre-scored aluminium discs of appropriate thickness, separates the driver and driven sections and enables improved control of the shock-wave. Helium is used as the driver gas for these experiments.

Six PCB 113B24 piezoelectric pressure transducers mounted at different locations on the driven section to measure shock velocity and one Kistler 603B transducer on the end-wall, to record pressure-time profiles simultaneously during experiments. The measured velocity is used to calculate the post-shock conditions using ‘reflected shock’ routine from Gaseq [28]. The acceptable error for the measured pressures behind the reflected shock wave was limited to  $\pm 1$  bar of the target pressure and uncertainties in the IDT measurement is  $\sim 20\%$ . No pre-ignition pressure rise was observed in the experimental results. More information on the HPST uncertainties can be found in supplemental material.

Acetylene dissolved in acetone (min 98.5%) was purchased from BOC Ireland. Initially, the experiments were performed at all conditions without purifying the fuel. Subsequently an acetone filter was used and the experiments were repeated at  $\varphi = 2.0$  and  $P = 10$  bar. The other gases used for the experiments O<sub>2</sub> (99.99%), N<sub>2</sub> (99.99%), Ar (99.99%) and He (99.96%) have been purchased from BOC Ireland and used without further processing.

## **2.2 Rapid compression machine (PCFC RWTH Aachen)**

The PCFC RCM used in *this study* is a single-piston machine where the creviced piston is pneumatically driven and hydraulically stopped at the end of compression. The details on the construction, measurement procedure and the sensors used (dynamic: Kistler 6125C, type 'T' thermocouple, static pressure: STS ATM 1.ST) are available in the study of Hemken et al. [29] with the exception of the dynamic pressure sensor. The gases N<sub>2</sub> ( $\geq 99.95\%$ ), Ar ( $\geq 99.996\%$ ), and O<sub>2</sub> ( $\geq 99.995\%$ ) used for the mixture preparation were supplied from Westfalen AG and Praxair. The fuel acetylene dissolved with acetone has a purity of 99.0% (Westfalen AG) and the acetylene without acetone has a purity  $\geq 99.6\%$  (Linde AG). The compressed temperature conditions were calculated using the isentropic compression and expansion routine from Gaseq [28]. For a given condition, the measured IDTs are reproducible within 15%, and the experimental uncertainty in the compressed temperature is within  $\pm 5$  K, as calculated using the procedure explained in [30]. As in previous studies [29-31], the IDTs are simulated with an effective volume profile accounting for the compression phase and heat loss after compression. Both HPST and RCM experimental data and sample pressure traces can be found in Supplemental material.

Table 1: Synopsis of experimental conditions studied at NUIG HPST and RWTH RCM.

*\*Repeated to check acetone effect*

$\phi$	C <sub>2</sub> H <sub>2</sub>	O <sub>2</sub>	N <sub>2</sub>	Ar	$p$ (bar)	% dilution
<b>1.0</b>	0.077	0.194	0.729	0.000	10, 20 and 30	73
<b>1.0</b>	0.040	0.100	0.430	0.430	10	86
<b>1.0</b>	0.010	0.026	0.482	0.482	10	96
<b>0.5</b>	0.040	0.202	0.758	0.000	10	76
<b>2.0*</b>	0.144	0.180	0.676	0.000	10	68

### 2.3 Constant-volume vessel (TAMU)

Centrally ignited spherical flame tests for acetylene-air mixtures were conducted at 1 and 2 atm at room temperature for equivalence ratios of 0.6–2.0. The experimental facility is a constant-volume cylindrical vessel with 5-inch-diameter (12.7 cm) viewing windows for Schlieren imaging. Further details on the new facility are provided by Morones et al. [32]. A high-speed camera recorded each test at 25,000 fps. LBV was extrapolated using nonlinear method I. Representative Schlieren images from *this study* are shown as Supplemental material. The stated uncertainty in the LBV measurements for the present study is  $\pm 5\%$ . Gas mixtures were made according to Dalton’s law of partial pressures. The mixtures were composed of atomic absorption grade acetylene and air, using a ratio of 21% O<sub>2</sub> to 79% N<sub>2</sub> to represent atmospheric air at standard conditions. To ensure that the acetylene did not become unstable and decompose during the filling process, each component of each mixture was added to the vessel at a low flow rate. The rate of pressure rise on filling was maintained below approximately 1 Torr s<sup>-1</sup> throughout each test. The temperature of the gas inside the vessel was monitored and maintained within 1.5 °C of the initial temperature throughout the entirety of the filling process for each test.

The acetylene used in *this study* was dissolved in 5 mol% acetone in the cylinder, as has been the global standard in the gas supply industry for decades. The method of purifying acetylene using activated carbon purifiers has been implemented previously with success

[33]. As the activated carbon adsorbed acetone, the effectiveness of the purifiers to remove acetone vapor from the acetylene decreased. Therefore, the purifiers were regularly replaced between tests to maintain a pure supply of acetylene.

#### **2.4 Spherical combustion vessel (ITV RWTH Aachen)**

A spherical vessel with 100-mm internal diameter equipped with 50-mm diameter quartz windows for optical access, was employed to measure LBVs for pure acetylene and acetylene externally doped with 5 mol% acetone at 1 atm and 298 K for  $\phi = 0.8$ –2.0. The outward location of the propagating flames is Schlieren imaged using a dual-field-lens arrangement. Images were taken by a LaVision High-SpeedStar 6 CMOS camera, at 25,000 fps with a resolution of 10.67 pixel/mm and a shutter speed of 1/338,000 s. LBV was extrapolated using nonlinear method by Kelley et al. [34]. The representative Schlieren images from *this study* can be found as Supplemental material.

The fuel mixture for several consecutive measurements is externally prepared in a mixing vessel using the partial pressure method and transferred to the combustion chamber via tubing. The whole arrangement is maintained at a temperature, to ensure no condensation of the fuel. Fuel/air mixtures were prepared with compressed air, which consists of 20.94% O<sub>2</sub>, 78.13% N<sub>2</sub> and 0.93% Ar, and solvent free acetylene, as used before in the RCM measurements. Partial pressures are tracked during mixture preparation using temperature-compensated pressure transducers of type Keller Series 35 X HTC. Acetone-doped mixtures were prepared by measuring the amount of acetone gravimetrically and injecting the fuel into the mixing vessel using a syringe. Thus, the risk of fuel decomposition due to the heated mixing environment can be reduced by shortened residence times. The overall mixture composition remains partial pressure controlled by adjusting acetylene and air partial pressures according to the pressure difference of injected acetone.

After the mix is allowed to settle in the combustion chamber, it is ignited at the mid-point of the vessel, using an external spark plug. The experimental uncertainty in the LBV is found to be less than 5%.

### 3. Results and Discussion

The experimental conditions were selected to provide new IDTs for acetylene/air oxidation at elevated pressures over the range of conditions never explored. The LBV experiments were performed at TAMU and RWTH Aachen, at  $0.6 \leq \phi \leq 2.0$  and  $P = 1$  and 2 atm and  $T = 298$  K. Moreover, the influence of acetone contamination on acetylene IDTs and LBVs has been explored. For all simulations, Chemkin-Pro [35] was used.

#### 3.1 Influence of acetone presence on acetylene IDTs and LBVs

Table 2 summarizes the various methods employed in different laboratories to study pure  $C_2H_2$ . Figure 2(a) compares IDTs for pure  $C_2H_2$  and  $C_2H_2$  dissolved in acetone, for the  $\phi = 2.0$  at 10 bar. No variation in IDTs is observed among the two fuels, which is further supported by the model predictions (acetone sub-mechanism from AramcoMech2.0 is combined with the Glarborg Mechanism). Figure 2(b) compares the LBVs of pure  $C_2H_2$  and  $C_2H_2$  dissolved in acetone, at 1 atm and 298 K, from two laboratories.

Table 2: The purification methods employed in different laboratories to study pure acetylene

Experiment	Lab	Purification method		% pure acetylene
IDT	NUIG	Filter (Perkin Elmer)	Balston filter (N9301399)	99.9 %
	RWTH Aachen (PCFC)	None	acetone free acetylene	> 99.6 %
LBV	TAMU	Filter (Matheson)	activated carbon purifiers (450B)	99.5 %
	RWTH Aachen (ITV)	None	acetone free acetylene	> 99.6 %

The Pure acetylene LBVs from TAMU are consistently higher than those of RWTH for  $0.6 \leq \phi \leq 2.0$  (peak LBV difference of 14.8 cm/s at  $\phi = 1.4$ ). However, the LBVs for acetylene dissolved in acetone agree well with one another in  $1.0 \leq \phi \leq 2.0$ . The difference in the measured peak LBVs of pure acetylene and acetylene dissolved in acetone at  $\phi = 1.4$  is 11.5 and 23.9 cm/s for RWTH and TAMU respectively. The experimental findings in *this study* confirm that acetone presence affects acetylene LBVs, which is reaffirmed by the modelling results. As shown in Fig. 2(b), with an increase in the molar concentration of acetone (1.0, 5.0 and 8.0%) in acetylene, the LBVs predicted by AramcoMech2.0 [23] decrease.

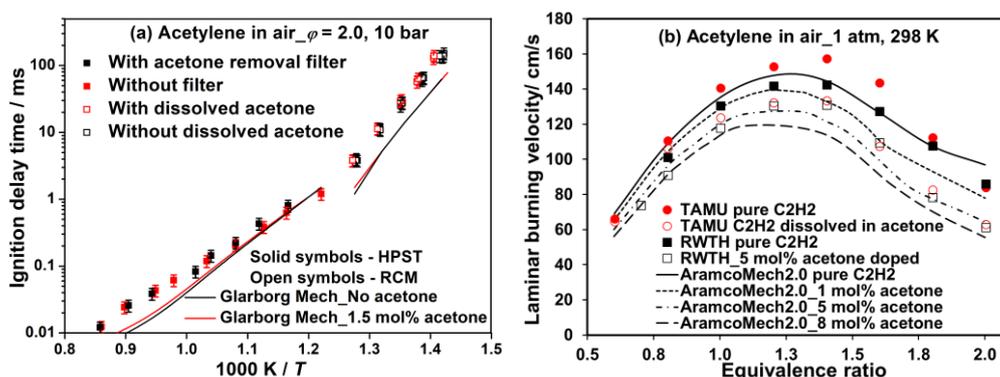


Fig. 2. Influence of dissolved acetone on acetylene IDTs and LBVs respectively.

### 3.2 Influence of pressure on acetylene IDTs

Figure 3 depicts the influence of pressure for stoichiometric acetylene/air mixtures for  $T = 700\text{--}1300$  K at  $P = 10, 20$  and 30 bar in a HPST and a RCM. The IDTs measured in the HPST show a minimal effect of pressure, but in the RCM regime, IDTs show a greater dependence on pressure. At lower temperatures, the IDTs can be seen to decrease with increasing pressure. The acetylene IDTs shows a strong Arrhenius behaviour across the temperature range investigated, with no negative temperature coefficient (NTC) at low-to-intermediate temperatures.

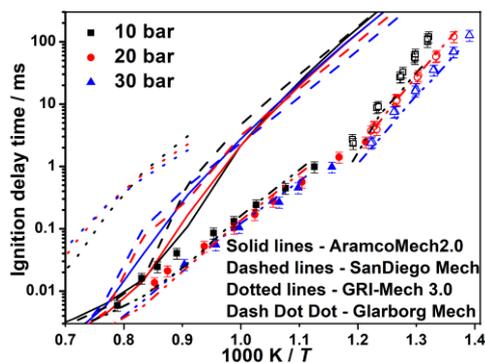


Fig. 3. Influence of pressure on acetylene IDTs at  $\phi = 1.0$ . Solid and open symbols correspond to HPST and RCM data, respectively.

Of particular interest is the lack of any negative pressure influence as predicted by three of the kinetic models [23-25]. With the exception of the Glarborg mechanism [26], all other models cannot predict the trend or the absolute IDTs of *this study*. Therefore, we use the Glarborg mechanism [26] for further interpretation of the data.

Figure 4 presents a rate of production (ROP) analysis performed using the Glarborg mechanism [26]. The analysis was made for stoichiometric acetylene/air at a temperature of 1021 K and at pressures of 10 and 30 bar. The ROP analyses using other models [23-25] at the same conditions is provided as Supplemental material. As expected, the quantity of unimolecular products formed from the consumption of acetylene increased with the pressure.

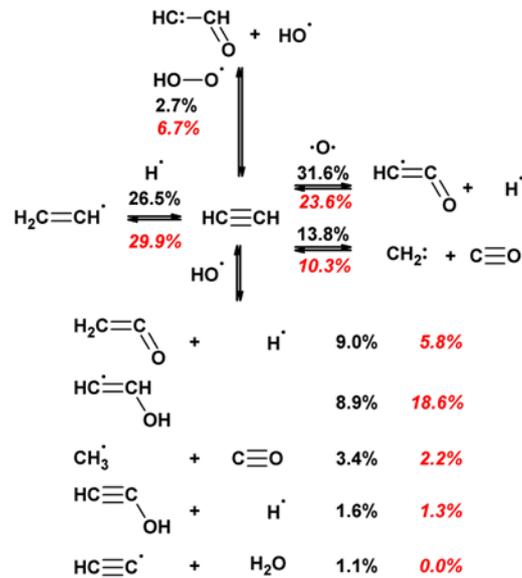


Fig. 4. Rate of production analysis for stoichiometric acetylene/air at 20% fuel consumption using Glarborg mechanism [24] at  $T = 1021\text{ K}$  and  $P = 10\text{ bar}$  (black),  $P = 30\text{ bar}$  (red).

Secondly, there is an increase in the amount of acetylene consumed through reaction with hydroperoxyl radicals to form triplet formylmethylene and hydroxyl radicals. Kéromnès et al. [22] previously showed an inverse dependence of hydrogen IDTs on pressure at intermediate temperatures (900–1250 K) which was attributed to competitive branching versus propagation pathways in the reaction of  $\dot{\text{H}}$  atoms with molecular oxygen. The branching pathway forms two reactive radicals ( $\dot{\text{O}}$  and  $\dot{\text{O}}\text{H}$ ), while propagation leads to the formation of one hydroperoxyl radical. These reactions are known to affect the prediction of all hydrocarbon IDTs.

In acetylene the existence, or not, of a branching versus chain-propagation mechanism also affects the simulations shown in Fig. 3 in which the Glarborg mechanism [26] is the only model to include the reaction of acetylene and hydroperoxyl radical forming triplet formylmethylene and hydroxyl radicals. This pathway promotes reactivity by producing two highly reactive radicals, with triplet formylmethylene subsequently reacting with molecular oxygen producing  $\dot{\text{O}}$  atoms which further react with acetylene, increasing reactivity. The absence of this reaction in the other models means that the IDTs are over estimated compared

to the new experimental data. The prominence of the inverse pressure dependence predictions by all other mechanisms is accentuated due to the over reliance of the acetylene chemistry on the underlying hydrogen oxidation reactions.

### 3.3 Influence of fuel-air equivalence ratio on IDTs

The influence of equivalence ratio on acetylene in air reactivity was investigated at 10 bar over fuel lean to fuel rich equivalence ratios, i.e. 0.5, 1.0 and 2.0, and is presented in Fig. 5. The two models closest to predicting the IDTs in Fig. 3 are used to predict the effect of equivalence ratio on acetylene IDTs in Fig. 5. The IDT decreases as the equivalence ratio increases for the temperatures 715–1250 K. In this case, both models capture the trend of the IDTs decreasing with increasing equivalence ratio. However, similar to the prediction of the effect of pressure, the Glarborg mechanism [26] best predicts the absolute IDTs at all three equivalence ratios. Both models predict that IDTs decrease with increasing equivalence ratios. This is a kinetic effect and is due to the increasing concentration of acetylene with increasing equivalence ratio in the temperature range 715–1250 K as the controlling chemistry depends on fuel concentration and not on O<sub>2</sub> concentration (which it does at high temperatures due to the importance of the reaction  $\dot{H} + O_2 = \ddot{O} + \dot{O}H$ ).

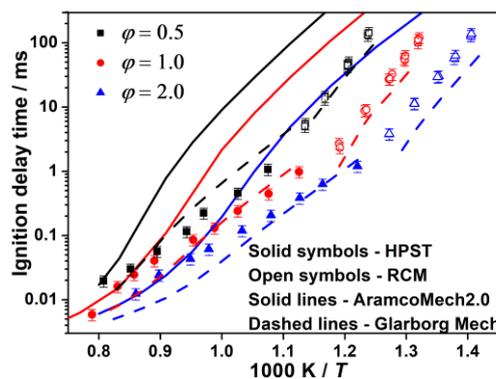


Fig. 5. Influence of fuel-air equivalence ratio on acetylene IDTs at 10 bar.

### 3.4 Influence of dilution on acetylene IDTs

IDT experiments for acetylene at 86% and 96% dilution were performed in the HPST and the RCM. Figure 6 compares the effect of the dilution on acetylene reactivity. As expected, IDTs increase with increasing diluent concentrations. The Glarborg mechanism [26] better reproduces the absolute measured IDTs, while AramcoMech2.0 [23] displays no effect of dilution at above 1000 K. For the two levels of dilution, AramcoMech2.0 [23] over-predicts IDTs at temperatures below 1100 K. This over prediction is due to the omission of the reaction of acetylene with hydroperoxyl radicals, which appears to be important over the range of dilutions studied.

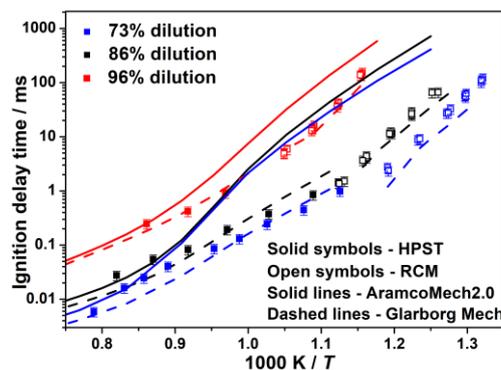


Fig. 6. Influence of dilution on acetylene IDTs at  $\phi = 1.0$  and 10 bar.

### 3.5 Laminar burning velocities

Figure 7(a) and (b) show the data from the current study (denoted as TAMU and RWTH) at 1 and 2 atm, plotted with the corresponding literature [12-14, 16]. As depicted in Fig. 7(a), the pure  $C_2H_2$  experiments performed independently at TAMU and RWTH have higher LBVs compared to the literature data. The current data for  $C_2H_2$  dissolved in acetone, agrees well with the data reported by Shen et al. [12], Jomaas et al. [14] and Ravi et al. [11] at 1 atm as shown in Fig. 7(a). Also note that the previous data measured at TAMU [11] were recorded without using an acetone-removal filter. This comparison strengthens the claim, that the presence of acetone decreases the LBVs of acetylene. Moreover, the peak LBV for the

literature data is around  $\phi = 1.3$ , while for the new data it is observed at  $\phi = 1.4$ . When compared to the literature data, the peak LBVs for pure acetylene from TAMU and RWTH increased by about 21 and 14 cm/s respectively. We conclude that the reason for the discrepancy in new experimental LBVs for pure  $C_2H_2$  with the literature data is due to the presence of acetone. AramcoMech2.0 generally under predicts the TAMU LBV data for pure  $C_2H_2$  and this divergence is seen to increase with equivalence ratio. This model agrees well with the RWTH data at  $1.4 \leq \phi \leq 2.0$  for pure  $C_2H_2$ . However, the Glarborg Mechanism predictions for pure  $C_2H_2$  are slower when compared to the LBVs from TAMU, but agrees well with the LBVs from RWTH, throughout the conditions investigated. As depicted in the Fig. 2(b), the difference in the peak LBV for *this study* and the existing data at 2 atm is about 27 cm/s. Similar to the 1 atm condition, AramcoMech2.0 predictions agree with the current study at 2 atm on the fuel-lean side, while they are slower on the fuel-rich side. The stark differences between the measured values in the literature and the present ones warrants a more detailed investigation for the acetylene-air LBV studies.

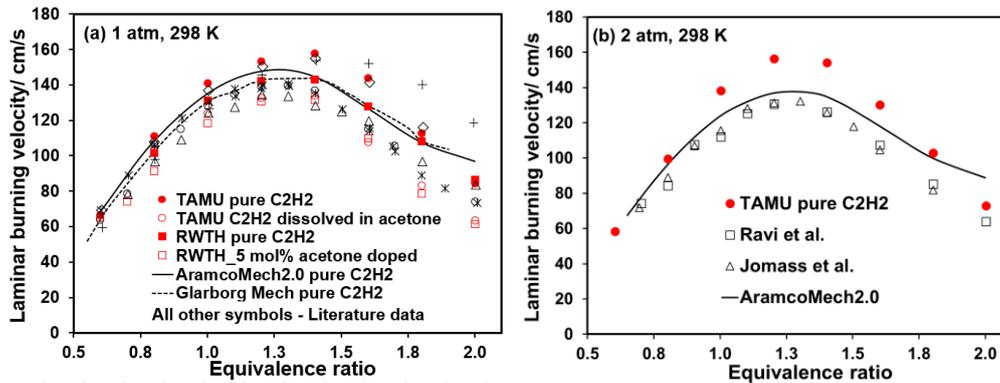


Fig. 7. Laminar burning velocities of acetylene/air at 1 and 2 atm respectively.

#### 4. Conclusions

*This study* presents new experimental measurements of IDTs and LBVs for acetylene oxidation using four independent experimental facilities. This is the first study to present IDTs for acetylene/air mixtures at pressure of 10, 20 and 30 bar. The effect of equivalence

ratio (0.5–2.0) was tested at a pressure of 10 bar. A wide range of temperatures (700–1300 K) was covered by using an RCM and a HPST. These IDTs were compared to predictions of four widely used literature kinetic models. Only the Glarborg mechanism was capable of reproducing the measured IDTs. A subsequent kinetic analysis using the Glarborg mechanism identified that the primary reason for the discrepancy between model predictions is due to the absence of the reaction of acetylene with hydroperoxyl radicals to form triplet formylmethylene and hydroxyl radicals. The IDTs exhibited no sensitivity to acetone presence, and this claim is further supported by the modelling results.

LBVs were measured independently at TAMU and RWTH Aachen. The measurements were performed with and without dissolved acetone. It was found that acetone affects LBVs, and this effect is reaffirmed by the modelling results. The measured LBVs for pure acetylene in both laboratories are faster compared to existing literature data, particularly under fuel-rich conditions. For the measurements of acetylene dissolved in acetone, the new data agrees well with those reported in the literature. This finding will impact upon the development of detailed chemical kinetic models for larger hydrocarbons as acetylene is produced as an intermediate for all larger hydrocarbons, and its abnormally fast LBVs means that it is a key component in the prediction of laminar burning velocities for larger hydrocarbons.

Both AramcoMech2.0 and the Glarborg Mechanism cannot accurately predict the current IDT and LBV results across all of the conditions investigated. The Glarborg Mechanism predicts the current IDT data reasonably well but is slower in predicting LBV across the conditions investigated. Meanwhile, AramcoMech2.0 does not predict the current IDT and LBV data at fuel-rich conditions but predicts LBV at fuel-lean conditions. Further work needs to be performed to improve the model predictions of the new data presented here.

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