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Laminar burning velocities of acetone in air at room and elevated temperatures

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HIGHLIGHTS

- We have determined laminar burning velocities of non-stretched acetone + air flames.
- The results show excellent reproducibility and resolve previous experimental discrepancies.
- The temperature dependence as a function of equivalence ratio was investigated.
- Kinetics modeling using a recently updated scheme shows agreement with experiments.

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ABSTRACT

Laminar burning velocities of acetone + air mixtures at initial gas mixture temperatures of 298, 318, 338 and 358 K are reported. Non-stretched flames were stabilized on a perforated plate burner at 1 atm, and laminar burning velocities were determined using the heat flux method, at conditions where the net heat loss from the flame to the burner is zero. The overall accuracy of the burning velocities was estimated to be better than ±1.0 cm s^{-1}. Very good reproducibility of the results and excellent agreement with modeling using a recently updated chemical kinetic model brings confidence in the validity of the reported results. Previous determinations of laminar burning velocities for acetone have provided inconsistent results. In the present work it is suggested that this can in part be attributed to the chemically aggressive nature of acetone.

1. Introduction

A fundamental property of a combustible mixture is its laminar burning velocity, the speed at which the flame front moves relative to the fresh gas. Laminar burning velocities are invaluable in the validation of combustion models and thus in understanding of the chemical kinetics. Flame speed variation with pressure and temperature is important for the development of combustion devices, while laminar burning velocities at ambient conditions can be used in the intercomparison of results between different labs and methodologies, and for model development.

Acetone is an important reaction intermediate in the oxidation of hydrocarbons in flames as well as in the atmosphere. As it reacts with available radicals like hydroxyl or hydrogen atoms, or undergo pyrolysis, it can form acetaldehyde, acetyl and acetonyl radicals [1]. Understanding the combustion properties and the chemical kinetics of acetone oxidation is essential for further development of kinetic models of hydrocarbon combustion. Determination of laminar burning velocities of acetone, as a function of equivalence ratio and temperature, is an important step towards reaching the goal of understanding its combustion chemistry.

Acetone is not only important as an intermediate produced in hydrocarbon oxidation, but is also of interest since it is used as a fuel tracer in laser induced fluorescence (LIF) measurements [2–4]. LIF can be used for determining both the distribution and the concentration of fuel in combustion systems, and since many fuels do not themselves absorb sufficiently in the wavelength range of relevance, compounds with well known spectral characteristics are added to the fuel as tracers. A limitation of the use of acetone as a fuel tracer is the fact that its chemical kinetics are not fully understood, and therefore its useful lifetime as a tracer is not well established [5]. Improved understanding of the combustion characteristics can be used to evaluate the usefulness of acetone as a fuel tracer.

In recent years several experimental studies of laminar burning velocity of acetone + air have been reported [5–9]. Earlier results [10–12] showed significant inconsistency that was in part attributed to the lack of stretch correction [9]. A summary of available experimental data on laminar burning velocities of acetone + air mixtures is given in Table 1, including studies published in peer reviewed journals [5,7,9,10,12] and from other sources [6,8,11,13].

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Table 1
Summary of measurements of laminar burning velocities of acetone + air flames.

T (K)	P (atm)	ϕ	Method	Year	Reference
298	1	0.7–1.2	Bunsen	1959	[10]
298	1	1–1.55	Bunsen	1962	[11]
296–520	0.4–8.5	1.0	Bomb	1981	[12]
298	1	0.9–1.6	Bomb	2007	[6]
298	1	0.7–1.7	Bomb	2008	[9,13]
298	1	0.8–1.5	Bomb	2009	[7]
298–358	1	0.7–1.6	Heat flux	2009	[8]
298	1	0.8–1.4	Stagnation jet	2011	[5]
298–358	1	0.7–1.4	Heat flux		This work

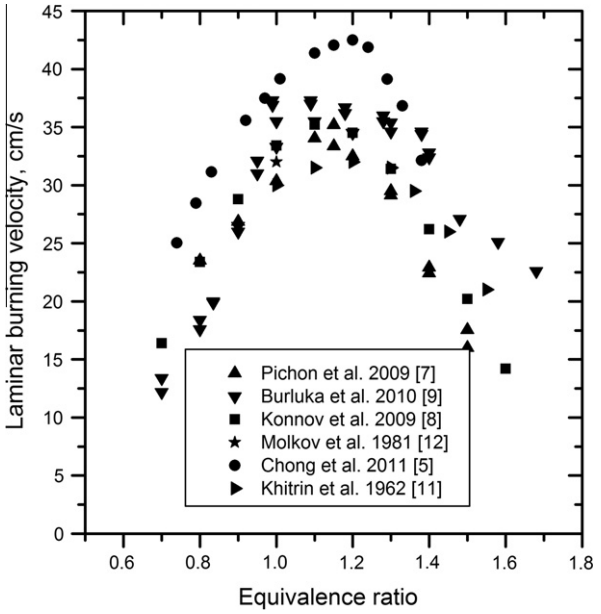

Fig. 1. Laminar burning velocities of acetone + air mixtures; literature data and results from the present study at atmospheric pressure and room temperature (298 K).

Literature data at 298 K and 1 atm are presented in Fig. 1 where a significant scatter in laminar burning velocities is apparent. Even though about 50 years separate the first study from the most recent ones, and the fact that the more recent data can be expected to be more reliable since necessary corrections due to stretch effects have been included, the consistency between different studies has not improved. At all available equivalence ratios the scatter in laminar burning velocity is in the range 8–12 cm s^{-1}.

The studies reported by Black et al. [6] and Pichon et al. [7] are essentially from the same research group, performed using the same spherical bomb configuration with Schlieren imaging. The later study was performed because a detailed chemical kinetic model then under development could not be reconciled with the first set of experimental results, hampered by some unknown uncertainty in the experiments. The results of the later study [7] gave generally lower values on burning velocities, it showed significantly better agreement with the model. Also Burluka et al. [9] used a spherical bomb configuration, in combination with Schlieren imaging or pressure registration. The results by Pichon et al. [7], and Burluka et al. [9] show fairly good agreement at the lean side and both give a maximum burning velocity of about 35 cm s^{-1}, see Fig. 1. At the rich side Burluka et al. [9] give significantly higher values (by 5–10 cm s^{-1}), closer to the results by Black et al. [6]. Burluka et al. [9] report on lower reproducibility of the laminar burning velocities for acetone flames, compared to two other fuels investigated within the same study.

For the studies performed in spherical bombs strong non-linearities in the dependence of laminar burning velocity on stretch in the flame are reported. This results in uncertainties in the laminar burning velocities [9]. To resolve these discrepancies Konnov et al. [8] used the heat flux method where the laminar burning velocity is determined from a non-stretched flame. They found burning velocities at 298 K in a good agreement with the measurements of Pichon et al. [7] at lean and stoichiometric conditions, and slightly higher values at the rich side. These results were published in conference proceedings [8], but were never submitted for a journal publication since the authors believed that systematic malfunction of the heat flux installation could lead to significant underestimation of the burning velocities as described in [14].

The most recent study, by Chong and Hochgreb [5], gives significantly higher results at all equivalence ratios, clearly seen in Fig. 1. The method used was jet-wall stagnation flame combined with particle imaging velocimetry (PIV) technique, and the un-stretched laminar flame speed was determined by making a linear extrapolation to zero stretch rate.

One can conclude that although several studies agree on the composition for the maximum burning velocity of acetone, the scatter in the data are too large to draw any final conclusions. Well known complications related to corrections due to stretch effects are possible reasons for the discrepancies in experimental results, but does not explain the fact that the reproducibility of the results within the different studies is not satisfactory. Moreover, the difference between the "true" burning velocity and those found without stretch-correction, using linear or non-linear extrapolation should correlate with Markstein lengths of burning mixtures [15]. For relatively heavy fuels like acetone, decreasing evolution of the Markstein length should be expected from lean toward rich mixtures and therefore improved consistency of different experiments should be anticipated in rich flames. This is not observed in Fig. 1, thus stretch correction or absence of it is likely not the only reason of the data spread.

Modeling of the acetone laminar burning velocities was attempted by Pichon et al. [7], Burluka et al. [9] and Chong and Hochgreb [5]. The modeling studies do not agree with the corresponding experimental studies, nor with each other. The model of Pichon et al. [7] reproduce their experimental results at the rich side very well, but fail on the lean side, and in predicting the position of the maximum. Burluka et al. [9] used an extended Konnov 0.5 model, which overpredicts the burning velocity of that study at the lean side, and around the maximum. At the lean side the modeling and the experimental results are within a few cm s^{-1}, while around unit stoichiometry and at the rich side the difference is up to 10 cm s^{-1}.

Chong and Hochgreb [5] model their results using GriMech 3.0 with a sub-mechanism for acetone added, and with some relevant reaction rates updated with recent values. The model show fairly good agreement with experimental results from that study, but the calculated maximum value is shifted towards unit stoichiometry compared to their measurements. Detailed species profiles of rich and lean premixed acetone flames were reported by Li et al. [1]. The results have been modeled by Pichon et al. [7] and Chong and Hochgreb [5]. Both groups report on divergence between experiment and modeling, in particular when the temperature profile by Li et al. [1] was used. Results were improved by a drastically altered temperature profile.

From the inconsistencies both when comparing modeling and experimental results, and when comparing the spread in results from different models, one can conclude that the understanding of the underlying chemistry has so far been insufficient. In the present study experimental determination of laminar burning velocities of acetone + air at different initial gas mixture temperatures is performed using the heat flux method. This method