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# Experimental determination of counterflow ignition temperatures and laminar flame speeds of C<sub>2</sub>–C<sub>3</sub> hydrocarbons at atmospheric and elevated pressures

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## Abstract

Experimental data were acquired for: (1) the ignition temperatures of nitrogen–diluted ethylene and propylene by counterflowing heated air for various strain rates and system pressures up to 7 atm; (2) the laminar flame speeds of mixtures of air with acetylene, ethylene, ethane, propylene, and propane, deduced from an outwardly propagating spherical flame in a constant-pressure chamber, for extensive ranges of lean-to-rich equivalence ratio and system pressure up to 5 atm. These data, respectively, relevant for low- to intermediate-temperature ignition chemistry and high-temperature flame chemistry, were subsequently compared with calculated results using a literature C<sub>1</sub>–C<sub>3</sub> mechanism and an ethylene mechanism. Noticeable differences were observed in the comparison for both mechanisms, and sensitivity analyses were conducted to identify the reactions of importance.

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*Keywords:* Ignition temperature; Laminar flame speed; Reaction mechanism

## 1. Introduction

Recent activities in the development of comprehensive oxidation mechanisms of hydrocarbon fuels have demonstrated: (1) the usefulness of such global flame response parameters as laminar flame speeds and ignition temperatures in mechanism validation and development; (2) the importance that such data are acquired from experimental flame/flow configurations that are aerodynamically clean and well-defined; and (3) the need that these mechanisms are comprehensive in their cov-

erage of the thermodynamic range of the combustible and the combustion environment, and hierarchical in the complexity of the fuel species. In particular, extensive laminar flame speed and ignition temperature data, at atmospheric as well as elevated pressures, have been acquired for the simplest fuel species, namely hydrogen and methane. These data have proven useful in mechanism development, for example, that of GRI-Mech for methane oxidation.

Comparatively fewer data have been reported for the hierarchically more complex C<sub>2</sub> and C<sub>3</sub> hydrocarbons. Specifically, ignition temperatures in the nonpremixed counterflow were measured by Fotache et al. [1] for ethane and propane from 1 to 7 atm. However, there do not exist any diffu-

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sive ignition data for the important olefin species. There are comparably more data on the laminar flame speeds, mostly by Egolfopoulos and co-workers [2–4], Faeth and co-workers [5,6], and Law and co-workers [2,3,7,8], as far as the recent measurements are concerned. However, since most of these data are from only one or two sources, the accuracy of the data cannot be adequately assessed. A notable example is the ethylene flame speed data at 1 atm, reported in [2]. These data were obtained by using the counterflow flame technique, with linear extrapolation to eliminate the strain rate effect. It is now recognized that linear extrapolation could result in flame speeds that are higher than those obtained by using either the more rigorous nonlinear extrapolation procedure [6–8] or for flame systems in which such an effect is either minimized [3], or does not exist [4]. Indeed, subsequent data from [6] show substantially lower values for the flame speed.

It is important to recognize that moderate extents of error in the laminar flame speed could result in noticeable differences in the mechanism developed, as is the case with methane oxidation in GRI-Mech. As far as the ethylene mechanism is concerned, the data of [2] have recently been used as one of the target points for optimization in developing a  $C_1$ – $C_3$  mechanism [9] that is being extensively adopted in various aspects of combustion studies. Since the accuracy of the developed mechanism must necessarily depend on the corresponding accuracy of its target points, and recognizing the importance of ethylene as a fuel by itself, as well as a key intermediate in the oxidation of other hydrocarbons, additional, independent measurements are essential, even if only to provide support to the accuracy of the newer data from [6].

In view of the above considerations, the primary objective of the present study was to acquire additional data on the ignition temperatures in nonpremixed counterflows and the laminar flame speeds of most of the  $C_2$ – $C_3$  hydrocarbons. These data cover the regimes of high-temperature oxidation in flames and low- to intermediate-temperature oxidation relevant for ignition, in premixed as well as nonpremixed situations, and with substantial pressure variations. The fairly comprehensive nature of the present experimentation is to be noted.

An additional objective of the present study was to compare the data obtained with those calculated by using selected mechanisms in the literature. However, in view of the large number of mechanisms available in the literature, and since it is also not the purpose of the present study to evaluate all the available mechanisms, the aim of the comparison was simply to provide an indication of the regimes of deficiency in some of these mechanisms, and through it stimulate further research towards their improvement.

In the following two sections, we shall, respectively, present the determination of the ignition temperatures and laminar flame speeds, with each section containing the experimental and computational methodologies, the experimental data, and the comparison between experiment and calculation. Linkage between the two studies is through the use of the same kinetic mechanisms, and their essential and combined utility in the development of comprehensive mechanisms.

## 2. Determination of ignition temperature in non-premixed counterflow

### 2.1. Experimental and computational specifications

The counterflow was generated from two axially aligned, opposing quartz tubes (20 mm inner diameter) that were separated by one tube diameter and housed in a variable-pressure chamber filled with nitrogen [1]. Air and nitrogen–diluted fuel were issued from the upper and lower tubes, respectively. Both burners were surrounded by nitrogen co-flows to improve flow stability, minimize radial temperature gradients, and isolate the reactants from the environment [1]. Air was heated by a silicon carbide heater located co-axially in the upper flow, and the temperature was regulated by a proportional-integral-derivative temperature controller. The flow rates of the fuel/nitrogen mixture and air were set using mass flow controllers (Teledyne Hastings) so that the stagnation surface was midway between the burner tubes.

Ignition of the diffusion flame was induced by gradually increasing the temperature of the air stream. The flame was then extinguished by reducing the fuel concentration and the velocity field corresponding to the incipient ignition state was measured by a two-component laser doppler velocimetry (LDV) system with frequency shifting (Dantec). Strain rates were determined by the axial velocity gradient on the oxidizer side of the stagnation surface. The temperature at the oxidizer exit was recorded using a K-type thermocouple with a bead diameter of about 180  $\mu\text{m}$ . This temperature was corrected for radiative/convective heat transfer [1], with an estimated maximum uncertainty of  $\pm 30$  K. The resulting temperature was the ignition temperature reported herein. This uncertainty constitutes the *absolute* error bars used in comparing the calculated and measured results. It must, however, be pointed out that the qualitative trend of the data is influenced mainly by the *relative* error, which ranges between  $\pm 2$  and  $\pm 5$  K and represents the repeatability of our experimental data.

Ignition calculations were performed using the flame continuation method of Nishioka et al. [10] with detailed transport and chemistry [11,12].

The kinetic models used are the optimized mechanism for  $C_1$ – $C_3$  [9] and the ethylene ignition mechanism of Varatharajan and Williams [13], which we shall refer to as the Q- and VW-mechanisms, respectively. The calculations determined steady state solutions at different hot boundary temperatures assuming potential flow, and the peak mole fraction of hydrogen atom was used to monitor the system response. The ignition temperature was defined as the hot boundary temperature at the turning point of the resulting S-curve. Due to the large amount of species, the grids were refined to the extent that the variation of calculated ignition temperature is less than 1 K. We note in passing that since ignition is mainly governed by the local velocity gradient immediately upstream of the mixing layer on the oxidizer side, the use of the simple potential flow formulation adequately describes the ignition characteristics [1].

## 2.2. Results and discussion

### 2.2.1. Ethylene and propylene

The effects of strain rate on the ignition temperatures of ethylene and propylene are shown in Fig. 1. We first note that the ignition temperature increases with increasing strain rate as a consequence of reduced residence time, similar to the previous results [1,14] on ethane, propane, *n*-butane, isobutane, *n*-heptane, and isooctane. Second, the sensitivities to strain rate variations, represented by the gradients of these fairly straight curves, are comparable in magnitude for these two fuels, with propylene being slightly more sensitive ( $0.49 \text{ K s}$ ) than ethylene ( $0.38 \text{ K s}$ ). Furthermore, the ignition temperature of propylene is about 50 K higher than that of ethylene. For both fuels, the trend-wise agreement between the experimental data and numerical simulation using both the Q- and the VW-mechanism is good. Quantitatively, calculations using the VW-mechanism are much closer to

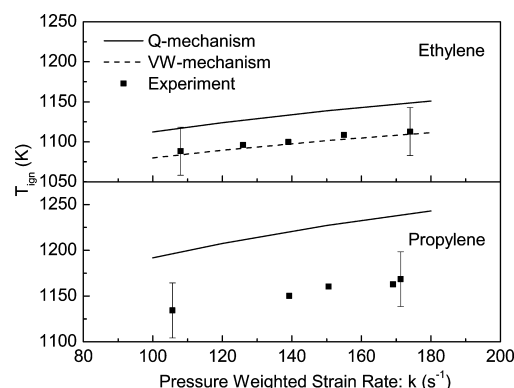


Fig. 1. Ignition temperatures as a function of strain rate for  $C_2H_4$  and  $C_3H_6$ . Conditions: 5.9% fuel in  $N_2$  and 3.1 atm.

the experimental data than those of the Q-mechanism for ethylene ignition, for which the prediction is slightly out of the absolute experimental error range. For propylene, the agreement between the calculated ignition temperature using the Q-mechanism and the experimental data worsens, with the former being about 70 K higher, which is quite beyond the absolute experimental error.

Figure 2 shows the effect of pressure on the ignition temperature of ethylene and propylene. The pressure-weighted strain rate was held constant to separate the influence of pressure variation on the ignition chemistry from the fluid dynamic variation of the strain rate [1,15]. It is seen that the ignition temperature for both fuels decreases with increasing pressure. This is reasonable in that radical build-up reactions are typically second order, and consequently speed up with increasing pressure because of the higher density. However, radical loss through diffusion is pressure insensitive because of the corresponding insensitivity of the pressure-weighted diffusion coefficient. This result also agrees with previous observations on alkanes [1,14]. It is further seen that, in general, the VW-mechanism agrees very well with the experimental results on ethylene over the pressure range of the present study. The Q-mechanism uniformly predicts higher ignition temperatures than the experimental data, having closer agreement for ethylene but larger deviation for propylene at higher pressures.

Sensitivity analysis of the S-curve [15], which determines its response in a region close to the ignition turning point to a perturbation in each of the reaction rates, i.e.,  $\partial \ln T_{ign} / \partial \ln A_i$ , was performed for both ethylene and propylene at three different pressures to identify the key reactions responsible for ignition, where  $T_{ign}$  is the ignition temperature, and  $A_i$  the pre-exponential factor for the  $i$ th reaction rate constant. The Q-mechanism

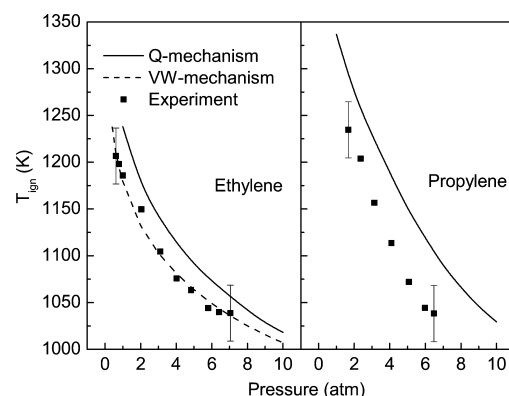


Fig. 2. Effect of pressure on ignition temperatures for  $C_2H_4$  and  $C_3H_6$ . Conditions: 5.9% fuel in  $N_2$  and  $k = 150 \text{ s}^{-1}$ .

was used for both ethylene and propylene, while the VW-mechanism was used for ethylene only. Space limitation, however, does not allow us to present the computed sensitivity coefficients. We shall therefore provide a summary of the results instead. First of all, the three cases share some similarities. The most sensitive reactions all include many of the  $\text{H}_2/\text{O}_2$ , CO, and  $\text{CH}_3$  reaction pathways. Second, at lower pressures, the most sensitive reactions to ignition are those which contribute to the radical pool formation, such as the chain branching reaction  $\text{H} + \text{O}_2 = \text{OH} + \text{O}$ . At higher pressures, radical pool formation is facilitated by the increased reactivity of the  $\text{HO}_2$  and  $\text{H}_2\text{O}_2$  radicals. Third, ignition is also very sensitive to reactions involving large fuel molecules attacked by radicals, such as  $\text{OH} + \text{C}_2\text{H}_4 = \text{C}_2\text{H}_3 + \text{H}_2\text{O}$  for ethylene, and  $\text{aC}_3\text{H}_5 + \text{HO}_2 = \text{OH} + \text{C}_2\text{H}_3 + \text{C}$  for propylene. Finally, comparing the results for ethylene ignition by both the Q- and the VW-mechanisms, it is found that the majority of the most sensitive reactions are identical. Thus, both mechanisms have included the necessary reaction pathways for ignition. The differences observed for the calculated ignition temperatures are therefore likely consequences of adopting different rate expression coefficients as well as including different minor reactions.

### 2.2.2. Ethane and propane

Since the Q-mechanism was developed for both  $\text{C}_1$ – $\text{C}_3$  alkenes and alkanes, it is interesting and necessary to extend the investigation to its performance for ethane and propane ignition. Figure 3 shows the experimental and calculated ignition temperatures, with the experimental data taken from previous studies [1]. It is seen that, for each fuel, the mechanism adequately captures the trend that ignition temperature decreases with increasing pressure. However, the predicted ignition temperatures are far beyond the experimental

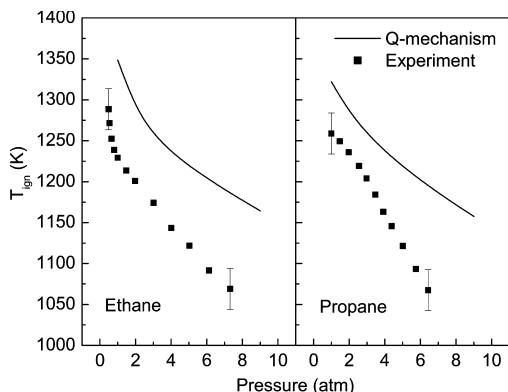


Fig. 3. Effect of pressure on ignition temperatures for  $\text{C}_2\text{H}_6$  and  $\text{C}_3\text{H}_8$ . Conditions: 5.9% fuel in  $\text{N}_2$  and  $k = 150 \text{ s}^{-1}$ .

absolute error of about  $\pm 25 \text{ K}$  [1], and the over-prediction increases at higher pressures, which is similar to the results for propylene ignition. Furthermore, the mechanism predicts that propane is easier to ignite than ethane at lower pressures, which is contrary to the experimental observation.

Sensitivity analysis shows that, once more, the ignition temperatures of ethane and propane are closely influenced by the  $\text{H}_2/\text{O}_2$ , CO, and  $\text{CH}_3$  reactions, since they are responsible for the radical pool formation and heat release. In addition, ignition is very sensitive to the large molecule breakdown reactions through the radical attack, such as  $\text{OH} + \text{C}_2\text{H}_4 = \text{C}_2\text{H}_3 + \text{H}_2\text{O}$  for ethane, and  $\text{aC}_3\text{H}_5 + \text{HO}_2 = \text{OH} + \text{C}_2\text{H}_3 + \text{C}$  for propane, which are the most sensitive reactions for the corresponding alkenes as well. These results imply that the oxidation of olefins is an essential component of the oxidation of paraffins, due to the hierarchical nature of the hydrocarbon oxidation chemistry.

### 2.2.3. Further comments on mechanisms

The above comparisons have shown that the Q-mechanism consistently over-predicts the non-premixed counterflow ignition temperatures for  $\text{C}_2\text{H}_4$ ,  $\text{C}_2\text{H}_6$ ,  $\text{C}_3\text{H}_6$ , and  $\text{C}_3\text{H}_8$ . Since this mechanism was optimized against 9 target shock tube ignition delay times for  $\text{CH}_4$ ,  $\text{a-C}_3\text{H}_4$ ,  $\text{p-C}_3\text{H}_4$ , and  $\text{C}_3\text{H}_8$  [9], the target species might not be extensive enough to include the entire  $\text{C}_1$ – $\text{C}_3$  hydrocarbon species. In addition, the temperature range of the shock tube experiments adopted by Qin et al. [9] is typically above 1400 K, which might not be low enough to adequately describe the low temperature kinetics, such as those prevailing at the counterflow ignition temperatures of about 1000–1200 K. Consequently, it is not unreasonable that the performance is not as satisfactory for the present counterflow ignition experiments involving other species and lower temperatures, despite the fact that the mechanism accurately predicts the shock tube ignition delay times for the target species [9]. By the same reasoning, since the VW-mechanism was particularly developed for  $\text{C}_2\text{H}_4$  ignition and detonation, and was verified against most shock tube ignition delay times, with the post-shock temperature ranging from 1000 to 2500 K, pressure from 0.5 to 100 bar, and equivalence ratio from 0.5 to 2 [13], the VW-mechanism is therefore expected to perform well.

## 3. Determination of laminar flame speeds

### 3.1. Experimental and computational specifications

The laminar flame speeds were determined using spark-ignited outwardly propagating flames (OPF), employing the dual-chamber design of Tse

et al. [16]. Premixtures of reactants were prepared in the inner chamber through partial pressures, while the outer chamber was filled with inert gases ( $N_2$  with either He or Ar). Two sleeves with holes that were offset relative to one another initially separated the two chambers. One sleeve was impulsively slid over the other so that the holes became aligned, and in the same instant the premixture was spark-ignited (adjustable spark duration between  $5 \mu s$  and  $1 ms$  [16]). Thus, the system allowed the inner chamber gas to pass through as the flame propagates. Due to the buffer effect of the outer chamber, which is 25 times larger, the subsequent pressure rise was less than 3% for the chamber [16]. At the small radii studied herein, the pressure rise is significantly smaller, resulting in a constant pressure combustion process. The flame propagation sequence was recorded using schlieren imaging and a high-speed digital motion camera at 8000 frames per second.

This arrangement allows for constant-pressure flame propagation with optical access, even in a high-pressure environment. Thus, by tracking the flame front, the flame radius can be determined as a function of time,  $r(t)$ . Since movement of the flame corresponds to that of its downstream boundary, and by allowing for stretch effects, the flame radius is found to vary with time  $t$  [17] according to

$$r + 2L_b \ln(r) = s_b^0 t + \text{constant}, \quad (1)$$

where  $s_b^0$  and  $L_b$  are the downstream laminar flame speed and the burned Markstein length, respectively. These two quantities can therefore be determined through a regression analysis of the experimental data,  $r(t)$ . Knowing  $s_b^0$ , the laminar flame speed (of the upstream boundary),  $s_u^0$ , is calculated by conservation of mass across the flame ( $\rho_u s_u^0 = \rho_b s_b^0$ ), where  $\rho$  is the density. There is no assumption of a flame sheet in the experimental procedure and data reduction, as we only determined the downstream flame speed, in the burned region, based on the history of the inner radius, and converted it to the unstretched upstream flame speed through the density ratio as described.

Computationally, the laminar flame speed was determined using a modified version of PREMIX [18]. In the present study, the Q- and the VW-mechanisms were used and the results were compared with the experimentally determined values.

### 3.2. Results and discussion

Experiments were performed for ethylene, ethane, propylene, and propane in air at pressures of 1, 2, and 5 atm, and for acetylene in air at 1 and 2 atm. At higher pressures, the onset of hydrodynamic instabilities prevented the flames from being smooth throughout the nominal tracking radius used for the regression analysis.

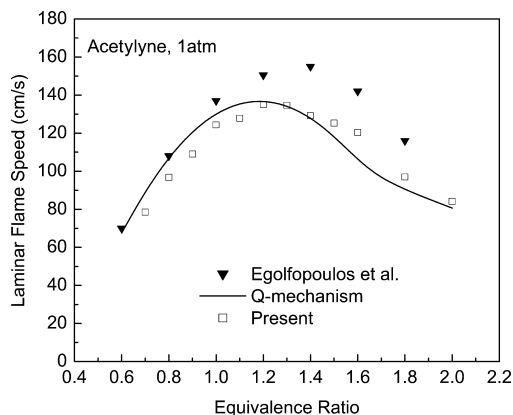


Fig. 4. Laminar flame speed of acetylene ( $C_2H_2$ ) in air at atmospheric conditions.

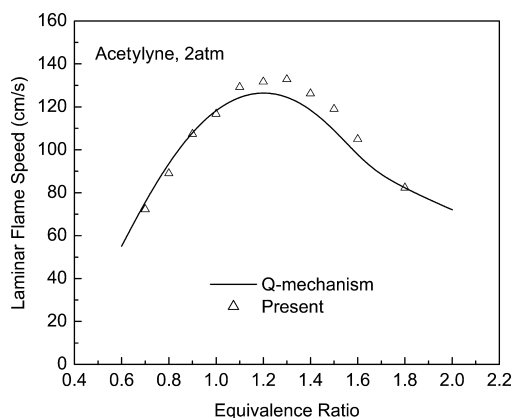


Fig. 5. Laminar flame speed of acetylene ( $C_2H_2$ ) in air at 2 atm.

The experimental and computed flame speeds for acetylene, ethylene, ethane, propylene, and propane are presented in Figs. 4–10. Due to the potential archival value of these carefully acquired experimental data, and for the sake of clarity, the data for both acetylene and ethylene at different pressures are plotted separately.

#### 3.2.1. Acetylene

Figures 4 and 5 show the results for acetylene at 1 and 2 atm, respectively. Figure 4 shows that the earlier experimental data of Egolfopoulos et al. [2] are consistently higher than the present values. Our initial concern with over-prediction due to the use of linear correction or stretch, as expressed for ethylene, can therefore be extended to apply to acetylene as well. It is further seen that the present experimental data are moderately close to the calculated values using the Q-mechanism, with slight over-prediction and under-pre-

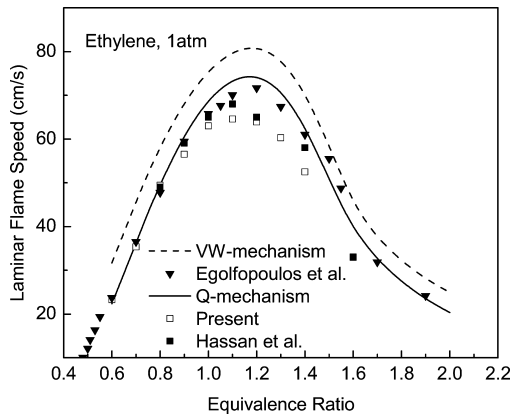


Fig. 6. Laminar flame speed of ethylene ( $C_2H_4$ ) in air at atmospheric conditions.

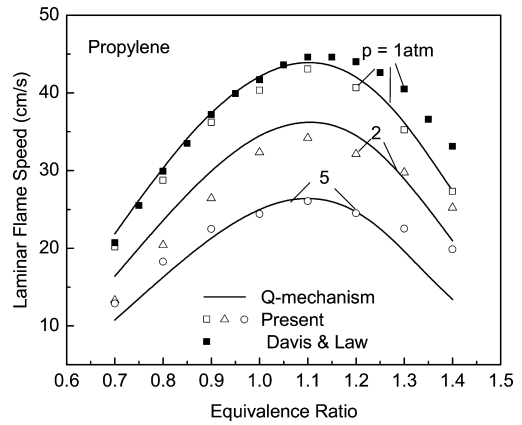


Fig. 9. Laminar flame speed of propylene ( $C_3H_6$ ) in air as a function of equivalence ratio and pressure.

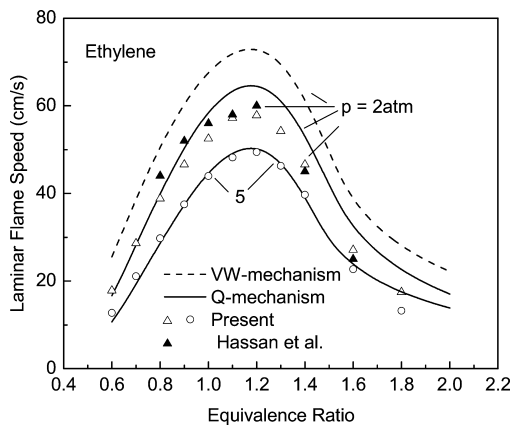


Fig. 7. Laminar flame speed of ethylene ( $C_2H_4$ ) in air at 2 and 5 atm.

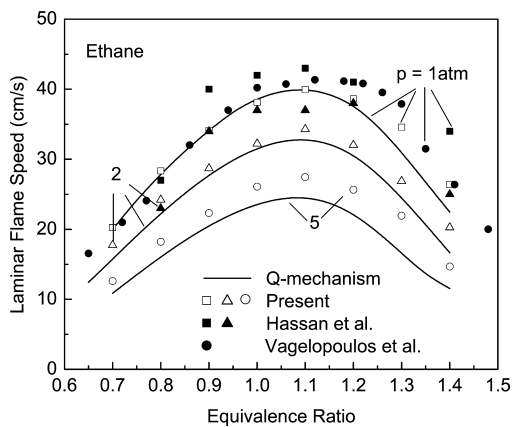


Fig. 8. Laminar flame speed of ethane ( $C_2H_6$ ) in air as a function of equivalence ratio and pressure.

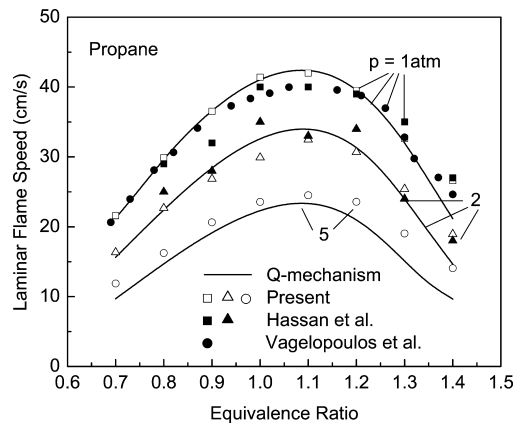


Fig. 10. Laminar flame speed of propane ( $C_3H_8$ ) in air as a function of equivalence ratio and pressure.

diction for the lean and rich mixtures, respectively. This agreement seems to be further improved at 2 atm, as shown in Fig. 5. Considering that acetylene was not a target fuel in the optimization studies of Qin et al. [9], the observed agreement is noteworthy.

### 3.2.2. Ethylene

Figure 6 shows the experimental data of Egolfopoulos et al. [2] and [6], the present experimental data, and computed values using the Q- and VW-mechanisms, all at 1 atm, while Fig. 7 shows results for 2 and 5 atm. It is seen that the present data agree well with those of Hassan et al. [6], but are substantially lower than those of Egolfopoulos et al. [2]. Furthermore, the 1 atm data of Egolfopoulos et al. [2] are comparable to the calculated values using the Q-mechanism, which is expected because these data were used as target points in the mechanism optimization. However,

precisely for this same reason, these calculated values substantially exceed the present experimental data, except for very lean mixtures. Figure 7 shows that the over-prediction persists at 2 atm, both in trend and in magnitude, while fairly close agreement is observed for the data at 5 atm.

Combining the results of acetylene and ethylene, it can be stated that the linearly extrapolated data of Egolfopoulos et al. [2] at 1 atm yield laminar flame speed values that are substantially higher than the correctly extrapolated values determined herein. Use of this earlier source has consequently biased the development of the  $C_1$ – $C_3$  reaction mechanism, leading to predictions of higher values for the flame speeds of ethylene at 1 atm. This effect, however, could be localized in that it seems to diminish for acetylene as well as for higher pressures. The very close agreement for ethylene at 5 atm must, however, be regarded as somewhat fortuitous.

Figures 6 and 7 in addition show that the VW-mechanism yields higher flame speeds for ethylene than the present experimental values. This is reasonable because the development of this ethylene mechanism again used the data of Egolfopoulos et al. [2]. Furthermore, it is seen that predictions using the VW-mechanism are higher than those of the Q-mechanism. Since the VW-mechanism also yields lower ignition temperatures, it might be suggested that this mechanism could embody factors that would lead to faster overall reaction rates.

### 3.2.3. Ethane, propane, and propylene

Figures 8–10 show the present experimental data and the calculated values using the Q-mechanism for ethane, propane, and propylene. Since the development of the Q-mechanism used the newer data of Vagelopoulos and Egolfopoulos [4] for ethane and propane, in which flame stretch was absent through an ingenious experimental arrangement, close agreement is observed for these two fuels. It is nevertheless interesting to note that the agreement for propylene is also close, even though propylene was not used in the mechanism development and it is structurally similar to ethylene, which is not described well by the mechanism. This again suggests that the faster reaction rates for atmospheric ethylene in the Q-mechanism could be moderately localized, to ethylene and acetylene for near-atmospheric situations.

## 4. Concluding remarks

In the present investigation, we have acquired data of high accuracy for the nonpremixed counterflow ignition temperatures and laminar flame speeds of the  $C_2$ – $C_3$  species of ethane, ethylene, acetylene, propane, and propylene. This informa-

tion is expected to be of value not only for practical use, but also for the partial validation and further development of kinetic mechanisms pertaining to these fuels. Its usefulness for the latter application is further noted by recognizing that the present data cover reaction situations ranging from the low- to intermediate-temperature ignition to the high-temperature flame propagation, in non-premixed and premixed systems, over extended ranges of reactant concentrations, and for atmospheric to moderately elevated pressures.

By comparing the present data with the calculated values using two existing mechanisms, it was demonstrated that the  $C_1$ – $C_3$  mechanism of Qin et al. [9] consistently yields results indicating stronger overall reactivity for all flame situations studied, while the ethylene mechanism of Varatharajan and Williams [13] yields higher flame speeds for ethylene. It is suggested that the observed stronger reactivity could be partly caused by the use of an earlier ethylene flame speed datum [2], obtained with some residue stretch effects, during the development of these mechanisms.

Recognizing the complexity of hydrocarbon oxidation processes, and the corresponding complexity of mechanism development, we close this presentation by noting the following. First, in guiding the development of mechanisms, experimental data of high fidelity are essential. As such, the earlier ethylene data of Egolfopoulos et al. [2], while considered to be rather adequate at the time of publication, in 1990, are now a possible source of error in the mechanism development. The reason being that current mechanism development demands greater overall accuracy as accuracies of the individual components of the mechanism have been tightened. Second, more targets are needed in mechanism development; especially in terms of the diversity of species, and even more so when optimization is involved. Third, any mechanism proposed must be subjected to extensive validation against experimental data. The validation should be conducted not only against the data on which the mechanism development is based, which are usually acquired from homogeneous systems, but it should also be applied to systems that have not been used in the development, such as the more complex but nevertheless well-defined diffusive systems of counterflow ignition and flame propagation, as attempted here.

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## Comments

David Smith, University of Leeds, UK. It is normal for  $T_{\text{ign}}$  and  $S_u$  to hinge on only a very few reactions

- Is that the case here?
- If so, what reactions?
- What does this tell us about the comparison of experimental and computed  $T_{\text{ign}}$  and  $S_u$ ?

*Reply.* If we interpret your question correctly, we agree and believe that there usually exist a few key reactions that qualitatively control the global response of a certain class of combustion phenomena within some ranges of the thermodynamic parameter space. For example, laminar flame speeds are mostly sensitive to small radical reactions, such as  $\text{HCO} + \text{M} = \text{H} + \text{CO} + \text{M}$ ,  $\text{CO} + \text{OH} = \text{CO}_2 + \text{H}$ , and  $\text{H} + \text{O}_2 = \text{OH} + \text{O}$ . On the other hand, for ignition under low to intermediate temperatures, the response is sensitive to two kinds of reactions. One is the  $\text{H} + \text{O}_2$  reaction, which is responsible for the radical pool formation. The other type is more specific to the fuel, such as  $\text{C}_2\text{H}_4 + \text{OH} = \text{C}_2\text{H}_3 + \text{H}_2\text{O}$  for  $\text{C}_2\text{H}_4$  ignition, and  $\text{aC}_3\text{H}_5 + \text{HO}_2 = \text{OH} + \text{C}_2\text{H}_3 + \text{CH}_2\text{O}$  for  $\text{C}_3\text{H}_6$  ignition.

At the minimum, a comparison of experimental and computed  $T_{\text{ign}}$  and  $S_u$  tells us the thermodynamic and system parametric ranges within which the chemical mechanism adopted works well or not. Thus while a close agreement does not necessarily validate the

adequacy and comprehensiveness of the mechanism, a poor agreement certainly indicates the presence of some deficiencies. Results of this nature provide useful guidance in the direction for further mechanism improvement.

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Suresh Aggarwal, University of Illinois at Chicago, USA. 1. Do you expect the same mechanism to perform well for predicting ignition temperatures (for nonpremixed mixtures) and laminar flame speeds (of premixed mixtures)?

2. Measured and predicted ignition temperatures typically differ by  $\sim 30$  K. Do you think this is within the experimental error?

*Reply 1.* Since the Q-mechanism was optimized against both ignition and flame speed data, it is reasonable to adopt it for the present comparisons. The purpose of our study is to scrutinize how well this mechanism describes our data, which has extensive parametric variation.

2. The typical difference between measured and predicted ignition temperatures is actually 80 K or even larger, which is well beyond the experimental of error about  $\pm 30$  K.