



HAL
open science

Measurements of flat-flame velocities of diethyl ether in air

Fiona Gillespie, Wayne K. Metcalfe, Patricia Dirrenberger, Olivier Herbinet, Pierre Alexandre Glaude, Frédérique Battin-Leclerc, Henry J. Curran

► **To cite this version:**

Fiona Gillespie, Wayne K. Metcalfe, Patricia Dirrenberger, Olivier Herbinet, Pierre Alexandre Glaude, et al.. Measurements of flat-flame velocities of diethyl ether in air. *Energy*, 2012, 43, pp.140-145. 10.1016/j.energy.2012.01.021 . hal-00715756

HAL Id: hal-00715756

<https://hal.science/hal-00715756v1>

Submitted on 9 Jul 2013

HAL is a multi-disciplinary open access archive for the deposit and dissemination of scientific research documents, whether they are published or not. The documents may come from teaching and research institutions in France or abroad, or from public or private research centers.

L'archive ouverte pluridisciplinaire **HAL**, est destinée au dépôt et à la diffusion de documents scientifiques de niveau recherche, publiés ou non, émanant des établissements d'enseignement et de recherche français ou étrangers, des laboratoires publics ou privés.

Measurements of flat-flame velocities of diethyl ether in air

Fiona Gillespie^{a,b}, Wayne K. Metcalfe^a, Patricia Dirrenberger^b, Olivier Herbinet^b, Pierre-Alexandre Glaude^b, Frédérique Battin-Leclerc^b, Henry J. Curran^a

^a Combustion Chemistry Centre, National University of Ireland, Galway, Ireland

^b Laboratoire Réactions et Génie des Procédés, CNRS, Université de Lorraine, Nancy, France

Abstract

This study presents new adiabatic laminar burning velocities of diethyl ether in air, measured on a flat-flame burner using the heat flux method. The experimental pressure was 1 atm and temperatures of the fresh gas mixture ranged from 298 to 398 K. Flame velocities were recorded at equivalence ratios from 0.55 to 1.60, for which stabilization of the flame was possible. The maximum laminar burning velocity was found at an equivalence ratio of 1.10 or 1.15 at different temperatures. These results are compared with experimental and computational data reported in the literature. The data reported in this study deviate significantly from previous experimental results and are well-predicted by a previously reported chemical kinetic mechanism.

Keywords

Laminar burning velocity; Diethyl ether; DEE; High temperature; Combustion

1. Introduction

Oxygenated biofuels are important in today's world due to a decline in oil and fossil fuels and an increase in CO₂ emissions and atmospheric pollution. Furthermore, as the price of fossil-derived fuels rises, focus is being drawn towards bio-derived fuels, the most common of which is bio-ethanol. Bio-ethanol is used predominantly in the United States and Brazil, in mixtures with gasoline of 10 and 85 vol. %; however, bio-ethanol is produced primarily from food sources (corn, sugarcane, etc.) and its energy output is not ideal [1] and [2]. Diethyl ether (DEE) is produced by dehydration of ethanol and is considered to be an excellent compression ignition fuel [3]. It has a cetane number above 125 and a larger heating value than ethanol.

Davoud and Hinshelwood [4] studied the thermal decomposition of DEE with focus on the amount of acetaldehyde present at each stage of the reaction. Freeman, Danby and Hinshelwood [5], [6], [7], [8] and [9] also studied the thermal decomposition of diethyl ether and focused on rate–pressure relations, effect of reaction conditions, nitric acid as an inhibitor, production of cyanides and production of ethanol. Waddington [10] investigated the gaseous oxidation of DEE at low temperatures and Laidler and McKenney [11] and [12] examined its pyrolysis from 833 to 893 K and 15–320 mmHg and the inhibition of pyrolysis by nitric acid from 833 to 913 K and 10–360 mmHg.

Diethyl ether has previously been investigated as an additive with common fuels in use in different engines. Mack et al. [13] experimentally investigated the addition of DEE to ethanol in a homogenous charge compression ignition (HCCI) engine in order to find a fuel blend that will elongate the combustion event and reduce the autoignition temperature relative to ethanol. However, they did not observe these desired results due to the similar nature of DEE and ethanol. Mosbach et al. [14] numerically simulated this data and predicted that the addition of diethyl ether accelerated combustion due to the greater ignitability of DEE. Miller Jothi et al. [15] explored the use of DEE as a cetane number improver for use with liquefied petroleum gas (LPG) in an HCCI engine. Their findings show a reduction in nitric oxide (NO), particulate matter (PM) and smoke emissions and an increase in hydrocarbon (HC) and carbon monoxide (CO) emissions compared to diesel fuel. Sudheesh and Mallikarjuna [16] added diethyl ether to biogas in an HCCI engine in order to improve ignition. This addition resulted in higher brake thermal efficiency and lower HC, NO and smoke emissions, however, an increase in CO emissions was observed. Cinar et al. [17] studied the effects of adding DEE to diesel fuel in an HCCI direct-injection engine and found that nitrogen oxide (NO_x) and soot emissions decreased and CO and HC emissions increased simultaneously. Iranmanesh et al. added DEE to diesel [18] and biodiesel [19] in a diesel engine and found that NO_x emissions decreased with addition to both fuels. However, they found that HC emissions increased with addition to biodiesel and carbon dioxide (CO₂) emissions increased with addition to diesel.

Recently, Yasunaga et al. [20] studied the oxidation and pyrolysis of DEE at high temperatures behind reflected shock waves. Their results showed that the most important reactions in the combustion of

DEE in a shock-tube are a four-centred elimination (reaction 1), C–O bond fission (reaction 2), and hydrogen abstraction to the secondary radical, C₂H₅OC₂H₄-s (reaction 3).



Agnew and Agnew [21] investigated the cool and two-stage flames of diethyl ether formed in flat-flame burners using infrared radiation techniques and observed emissions from excited formaldehyde in the range from 3200 to 5100 Å. Griffiths and Inomata [22] studied the oscillatory cool flames of diethyl ether in air experimentally and numerically to investigate the low temperature oxidation of diethyl ether, which, they found, was associated with the hydroperoxide CH₃CH(OOH)OC₂H₅.

Burning velocities of DEE have been measured by Gibbs and Calcote [23] using a Bunsen burner flame cone and the apex-cone method. Di et al. [24] and Zhang et al. [25] and [26] used a spherically propagating flame in a cylindrical vessel to obtain laminar burning velocities and study the combustion characteristics of diethyl ether. However no results have been reported for DEE flame velocities using the heat flux method.

This study presents new adiabatic laminar burning velocities of diethyl ether in air, measured on a flat-flame burner using the heat flux method [27]. The experimental pressure was 1 atm and initial temperatures of the fresh gas mixture ranged from 298 to 398 K. These results are compared with the experimental data of Gibbs and Calcote [23] and Di et al. [24], and simulations using the mechanism of Yasunaga et al. [20].

2. Experimental method

The heat flux method was first proposed by de Goey et al. [27] in 1993. This method is beneficial because stretching of the flame does not occur and therefore stretch correction or extrapolation of the data is not necessary. This particular apparatus has previously been used to measure laminar flame velocities of components of surrogate mixtures of natural gases [28].

In the flat-flame adiabatic burner, a brass burner plate, used to stabilize the unstretched flame, is mounted on a plenum mixing chamber, Fig. 1. The burner plate is 2 mm thick and 30 mm in

diameter. The plate is perforated with small holes of diameter 0.5 mm, with the pitch between them being 0.7 mm. Eight Type K thermocouples, of diameter 0.5 mm, are soldered to the plate surface at different distances and angles from the centre to the edge of the plate. The plenum chamber is encompassed by a thermostatic oil jacket, the temperature of which is set to the desired initial temperature of the unburned gas mixture. The circumference of the burner plate is heated with thermostatic oil set to 50 K above the temperature of the unburned gas mixture. In practice, if an initial temperature of 298 K is desired, the temperature of the plenum chamber is set to 298 K and that of the burner plate to 348 K. The oil is applied to the burner plate in order to maintain the plate at a constant temperature and to heat up the cooler unburned gas mixture as it flows through the plate, which compensates for the heat loss necessary to stabilize the flame.

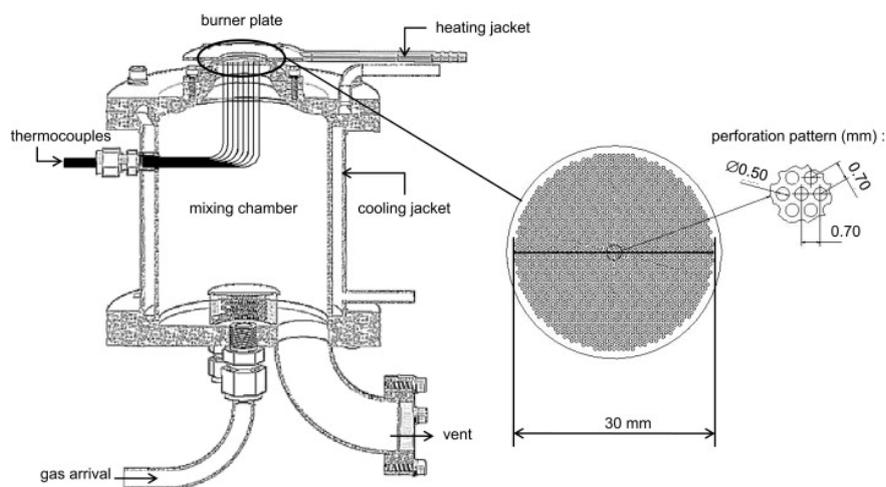


Fig. 1. Schematic of flat-flame adiabatic burner [28].

Flow rates for liquid compounds are measured using a Bronkhorst mini-CORI-FLOW Mass Flow Controller connected to a Controlled Evaporator Mixer (CEM). The CEM is connected to the plenum chamber using a duct which is wrapped with heating cable in order to keep the compound in the gaseous state as it enters the chamber. Temperature controllers indicate the temperature of the experimental setup at two locations: one below the chamber after the Mass Flow Controllers and one inside the chamber below the burner plate.

Flow rates for gaseous compounds are measured using Bronkhorst High-Tech Mass Flow Controllers (MFCs). At most conditions, the MFC used for oxygen has a maximum flow of 3 nL/min (normal litres per minute) while that used for nitrogen has a maximum flow of 15 nL/min. When the adiabatic flame burning velocity of a gas mixture is above a certain limit, specific to each different temperature tested, two MFCs are used to allow a sufficient flow of oxygen through the burner plate. Bronkhorst conversion coefficient factors are used to convert an MFC designed for nitrogen (with a maximum flow of 3 nL/min) for use with a flow of oxygen.

Adiabatic flame burning velocities in a flat-flame burner are measured using the radial temperature distribution on the surface of the burner plate. If the sum of the heat loss and heat gain is larger than zero, the gas velocity is lower than the adiabatic flame burning velocity. Thus, the centre of the burner plate is hotter than the circumference and the flame is stabilized under sub-adiabatic conditions. Conversely, if the sum of the heat loss and heat gain is lower than zero, the flame is stabilized under super-adiabatic conditions and the centre of the plate is cooler than the circumference. When the flow rate of the gas mixture is changed, an appropriate value of the gas velocity is found that will cancel out the net heat flux. Therefore, the heat loss from the flame to the burner plate is compensated by the heat flux from the burner plate to the unburned gas mixture. The radial temperature distribution in the burner plate is uniform and equal to the temperature of the heating jacket. At this point, the flame is adiabatic, the sum of the heat loss and heat gain from the flame is zero and the adiabatic burning velocity is measured.

Uncertainties in determination of the flame burning velocity are due to errors in:

- Mass flow measurements, with a maximum error of 0.5% per MFC, as given by the manufacturer, Bronkhorst, and a maximum global error in laminar flame velocity of 1.5%.
- The thermocouples, with an error of 0.2 cm s^{-1} in the laminar flame velocity. This error was measured by changing the gas flow rate by small amounts that did not affect the uniform temperature profile of the flame on the burner plate noticeably.
- Flame distortions, for example edge effects, with an error of 0.2 cm s^{-1} in the laminar flame velocity in the range of equivalence ratios studied. This error was measured similar to the error in the thermocouples.

Errors of around 1% were present when determining the equivalence ratio, ϕ , due to mass flow effects, as given by Bronkhorst. The temperature of the unburned gas mixture before and after it flowed through the plenum chamber was measured with a thermocouple. An error of 2 K was estimated. Errors in gas and liquid fuel purity were not significant as high purity compounds were used.

3. Results

3.1. Flat-flame velocities of diethyl ether

The apparatus has previously been validated with methane, which is described in detail by Dirrenberger et al. [28]. Diethyl ether was studied in air at a pressure of 1 atm, initial temperatures between 298 and 398 K and equivalence ratios from 0.55 to 1.60, Fig. 2. Error bars have been added to these data points. The adiabatic burning velocity increases sequentially with an increase in initial temperature. The maximum flame burning velocity is recorded at $\phi = 1.15$ at 398 and 378 K and at ϕ

= 1.10 at 388, 358, 328 and 298 K. It appears that the maximum burning velocities are shifting to the higher equivalence ratio of 1.15 at higher temperatures, but this is not the case for a temperature of 388 K. This may be due to uncertainties in the flame burning velocity. The adiabatic burning velocity measurements obtained are shown in Table 1.

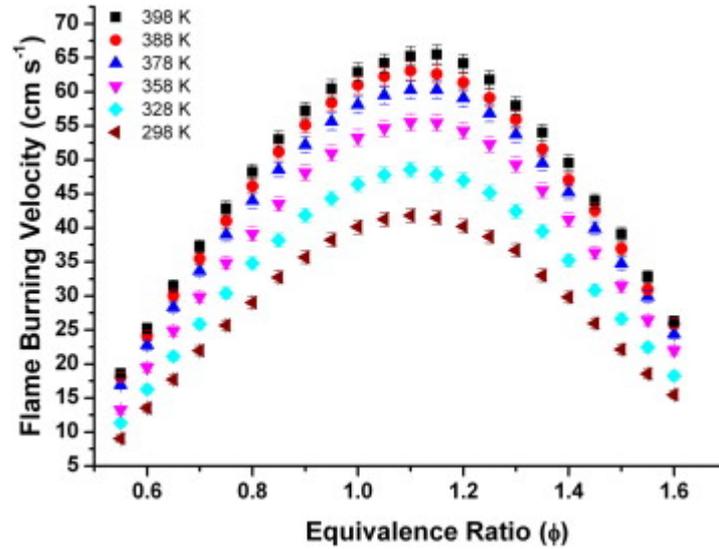


Fig. 2. Adiabatic burning velocities of diethyl ether.

Table 1. Adiabatic burning velocities (in cm s^{-1}) of diethyl ether obtained in the flat-flame burner. Maximum burning velocities at each equivalence ratio are in bold.

ϕ ($\pm 1\%$)	298 K (± 2 K)	328 K (± 2 K)	358 K (± 2 K)	378 K (± 2 K)	388 K (± 2 K)	398 K (± 2 K)
0.55	9.04 (± 0.54)	11.32 (± 0.57)	13.24 (± 0.60)	16.96 (± 0.65)	18.12 (± 0.67)	18.61 (± 0.68)
0.60	13.54 (± 0.60)	16.29 (± 0.64)	19.48 (± 0.69)	22.79 (± 0.74)	24.13 (± 0.76)	25.22 (± 0.78)
0.65	17.72 (± 0.67)	21.15 (± 0.72)	24.86 (± 0.77)	28.34 (± 0.83)	30.08 (± 0.85)	31.45 (± 0.87)
0.70	21.97 (± 0.73)	25.88 (± 0.79)	29.82 (± 0.85)	33.70 (± 0.91)	35.49 (± 0.93)	37.26 (± 0.96)
0.75	25.68 (± 0.79)	30.39 (± 0.86)	34.85 (± 0.92)	39.02 (± 0.99)	41.01 (± 1.02)	42.87 (± 1.04)
0.80	29.03 (± 0.84)	34.81 (± 0.92)	39.12 (± 0.99)	44.01 (± 1.06)	46.12 (± 1.09)	48.24 (± 1.12)
0.85	32.74 (± 0.89)	38.20 (± 0.97)	43.55 (± 1.05)	48.55 (± 1.13)	51.18 (± 1.17)	53.01 (± 1.20)
0.90	35.70 (± 0.94)	41.84 (± 1.03)	48.11 (± 1.12)	52.22 (± 1.18)	55.14 (± 1.23)	57.22 (± 1.26)
0.95	38.25 (± 0.97)	44.31 (± 1.06)	50.97 (± 1.16)	55.64 (± 1.23)	58.39 (± 1.28)	60.47 (± 1.31)
1.00	40.13 (± 1.00)	46.43 (± 1.10)	53.25 (± 1.20)	58.13 (± 1.27)	60.98 (± 1.31)	62.89 (± 1.34)
1.05	41.28 (± 1.02)	47.79 (± 1.12)	54.64 (± 1.22)	59.50 (± 1.29)	62.25 (± 1.33)	64.22 (± 1.36)
1.10	41.81 (± 1.03)	48.54 (± 1.13)	55.51 (± 1.23)	60.30 (± 1.30)	63.10 (± 1.35)	65.26 (± 1.38)
1.15	41.49 (± 1.02)	47.87 (± 1.12)	55.44 (± 1.23)	60.32 (± 1.30)	62.61 (± 1.34)	65.49 (± 1.38)
1.20	40.24 (± 1.00)	46.98 (± 1.10)	54.25 (± 1.21)	59.08 (± 1.29)	61.37 (± 1.32)	64.16 (± 1.36)
1.25	38.70 (± 0.98)	45.15 (± 1.08)	52.28 (± 1.18)	56.85 (± 1.25)	59.10 (± 1.29)	61.78 (± 1.33)
1.30	36.73 (± 0.95)	42.46 (± 1.04)	49.32 (± 1.14)	53.74 (± 1.21)	55.94 (± 1.24)	57.99 (± 1.27)
1.35	33.03 (± 0.90)	39.50 (± 0.99)	45.51 (± 1.08)	49.52 (± 1.14)	51.64 (± 1.17)	54.01 (± 1.21)
1.40	29.81 (± 0.85)	35.23 (± 0.93)	41.23 (± 1.02)	45.26 (± 1.08)	47.09 (± 1.11)	49.56 (± 1.14)
1.45	25.95 (± 0.79)	30.88 (± 0.86)	36.34 (± 0.95)	39.89 (± 1.00)	42.56 (± 1.04)	43.96 (± 1.06)
1.50	22.12 (± 0.73)	26.64 (± 0.80)	31.45 (± 0.87)	34.76 (± 0.92)	36.96 (± 0.95)	39.08 (± 0.99)
1.55	18.56 (± 0.68)	22.44 (± 0.74)	26.44 (± 0.80)	29.89 (± 0.85)	30.96 (± 0.86)	32.81 (± 0.89)
1.60	15.46 (± 0.63)	18.28 (± 0.67)	21.97 (± 0.73)	24.41 (± 0.77)	25.91 (± 0.79)	26.26 (± 0.79)

3.2. Comparison with literature data

In 1959, Gibbs and Calcote [23] measured the burning velocities of 77 different compounds in order to show the effect of molecular structure on these velocities. Burning velocities of diethyl ether were determined at 298 K and atmospheric pressure, Fig. 3. They found the maximum burning velocity to be at $\phi = 1.0$ with a value of 48.0 cm s^{-1} , which is in contrast with the results obtained in this study which show a maximum burning velocity of 41.81 cm s^{-1} at $\phi = 1.10$. This is due to the fact that Gibbs and Calcote did not take into account stretch correction of their flames, as most modern studies do. In addition, Davis and Law [29] have reported that the flames studied by Gibbs and Calcote [23] were non-adiabatic and non-equidiffusive, which are factors that have a great effect on the laminar flame burning velocity of the fuel. Therefore, their results are consistently different from those obtained with more modern techniques.

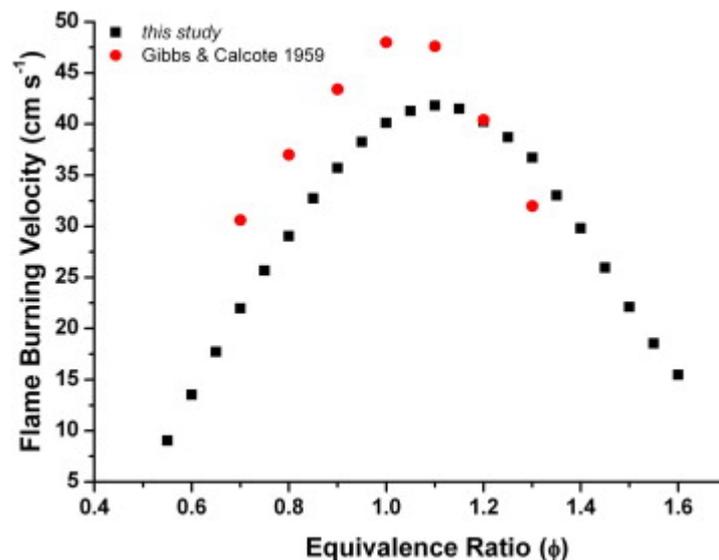


Fig. 3. Comparison of diethyl ether data obtained in this study with data obtained by Gibbs and Calcote [23] at 298 K.

Di et al. [24] measured laminar burning velocities of diethyl ether at different temperatures, pressures and equivalence ratios using spherically propagating flames in a combustion vessel. The maximum burning velocity at atmospheric pressure and at all temperatures is recorded at $\phi = 1.10$, which is comparable with measurements from this study and results simulated using the mechanism of Yasunaga et al. [20], Fig. 4. However, the results of Di et al. [24] are quite scattered and deviate significantly from the results obtained in this study and the simulated results, especially at high initial temperatures. Under lean conditions, velocities measured by Di et al. [24] are faster than those obtained in this study and the simulated results, whereas under rich conditions, velocities are slower than those in this study and the simulated results. Variations in these data sets may be due to the stretch correction necessary to acquire laminar flame velocities in combustion vessels with spherical flames. In the case of spherically propagating flames, two conditions occur which must be accounted

for [30]: the rise in pressure in the combustion vessel must be determined correctly and the equation used to measure flame velocities must be valid throughout this pressure rise.

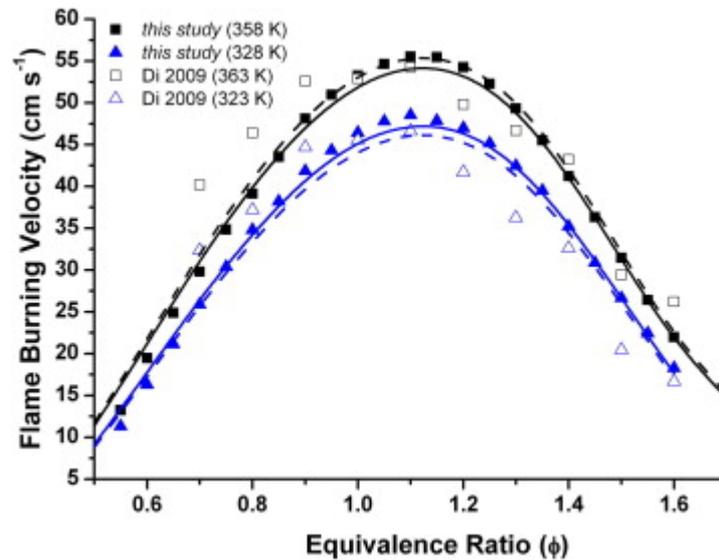


Fig. 4. Comparison of diethyl ether data obtained in this study at 328 and 358 K with data obtained by Di et al. [24] at 323 and 363 K. Results simulated using the mechanism of Yasunaga et al. [20]. Symbols: experiment; lines: simulation.

3.3. Comparison with model

Adiabatic flame velocity measurements obtained in this study were compared to simulated results obtained using the mechanism of Yasunaga et al. [20], updated with a new C₀–C₃ sub-mechanism in construction at the Combustion Chemistry Centre in NUI Galway, Fig. 5 and Fig. 6. The C₀–C₃ sub-mechanism is based on our previous work [31], [32] and [33], with the most recent updates described in [34] and [35]. The experimental results are well-predicted by the model and the overall trend in flame velocities is reproduced. Deviations between the simulated and the experimental results are within the limits of experimental errors. All simulations were performed using Chemkin-PRO [36].

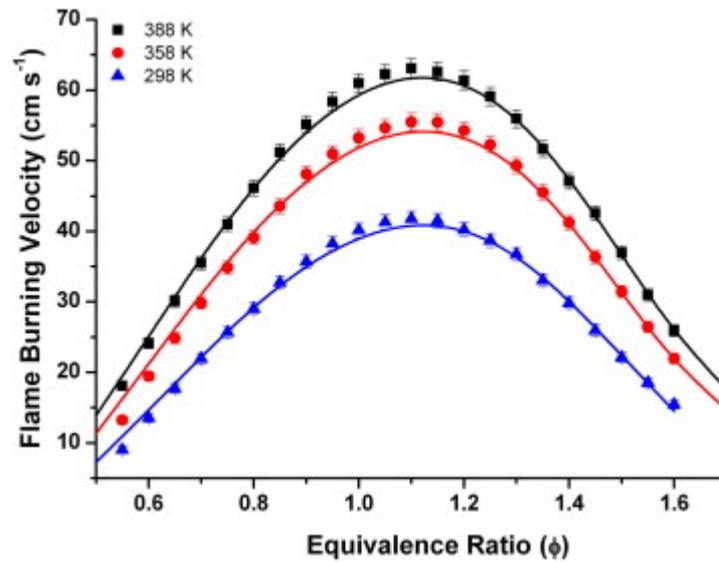


Fig. 5. Comparison of diethyl ether data obtained in this study with results simulated using the mechanism of Yasunaga et al. [20] at 298, 358 and 388 K. Symbols: experiment; lines: simulation.

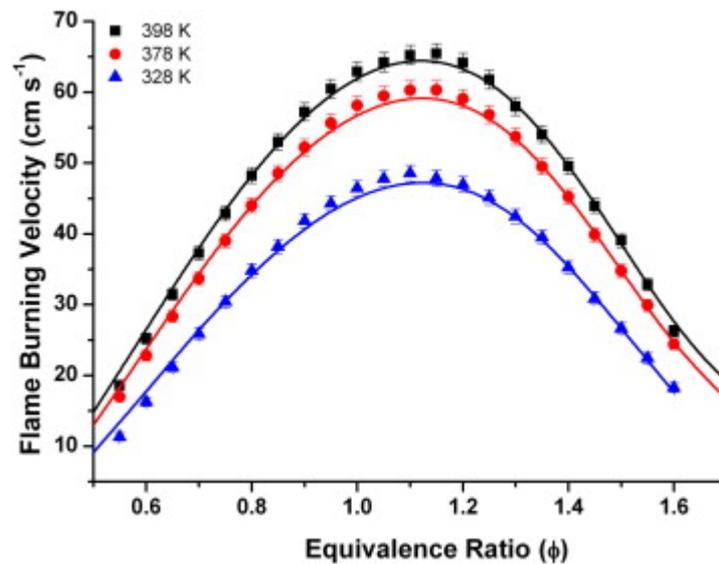


Fig. 6. Comparison of diethyl ether data obtained in this study with results simulated using the mechanism of Yasunaga et al. [20] at 328, 378 and 398 K. Symbols: experiment; lines: simulation.

Sensitivity analyses were performed using the sensitivity function available in Chemkin-PRO [36] and show the effect of a reaction on the flow rate, which corresponds to the burning velocity. These analyses were carried out at an equivalence ratio of 1.10 and an initial temperature of 298 K, Fig. 7, and at an equivalence ratio of 1.15 and an initial temperature of 398 K, Fig. 8. Reactions with negative sensitivity coefficients inhibit reactivity, while reactions with positive sensitivity coefficients promote reactivity. The chain branching reaction between hydrogen atom and molecular oxygen to

produce an oxygen atom and a hydroxyl radical is omitted for clarity and has a value of +0.406 at 298 K and $\phi = 1.10$ and a value of 0.411 at 398 K and $\phi = 1.15$. Of the 20 most important reactions, those with smaller molecules, such as methyl, ethyl and carbon monoxide, have the largest effect on the flame burning velocities of diethyl ether. It is important to note that only one reaction involving diethyl ether has a significant effect on flame burning velocities, that between diethyl ether and hydrogen atom to form hydrogen molecule and the secondary radical, $C_2H_5OC_2H_4\cdot$ s. The reaction between hydrogen atom and hydroxyl radical to produce water is the most inhibiting reaction at both conditions because it is in direct competition with the chain branching reaction to produce oxygen atom and hydroxyl radical.

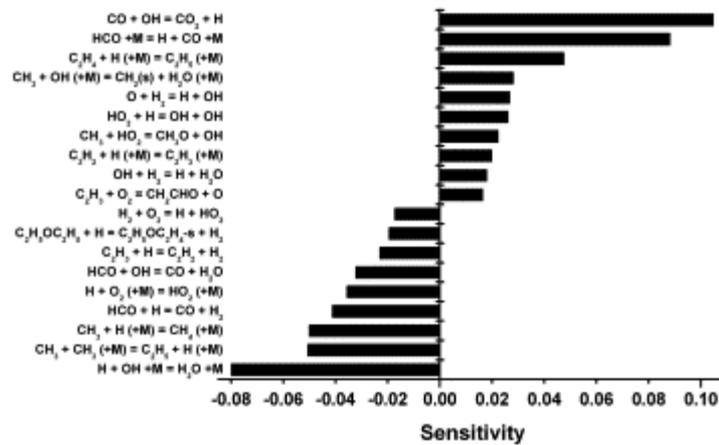


Fig. 7. Sensitivity coefficients showing the 20 most important reactions in diethyl ether flame burning velocities at 298 K and $\phi = 1.10$.

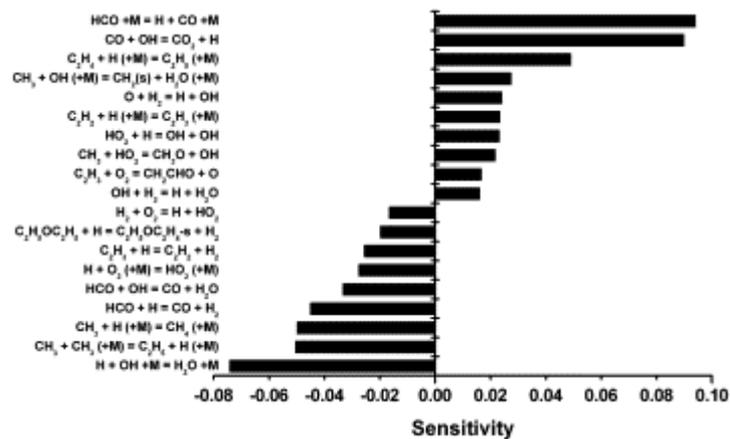


Fig. 8. Sensitivity coefficients showing the 20 most important reactions in diethyl ether flame burning velocities at 398 K and $\phi = 1.15$.

4. Conclusions

Adiabatic flame burning velocities of diethyl ether in air have been studied on a flat-flame burner at atmospheric pressure and six temperatures between 298 and 398 K. Equivalence ratios for these experiments ranged from 0.55 to 1.60. It was found that the adiabatic burning velocities increased with respect to temperature. The maximum flame velocity was reported to be at $\phi = 1.10$ at 298, 328, 358 and 388 K and at $\phi = 1.15$ at 378 and 398 K. It was suggested that the maximum velocities were shifting to $\phi = 1.15$ at higher temperatures, but this was not the case at 388 K, due to uncertainties. These results were compared with experimental results from the literature [23] and [24] and were found to deviate significantly. The results of Gibbs and Calcote [23] were non-adiabatic and non-equidiffusive and stretching of the flame was not accounted for. The results of Di et al. [24] differed from the findings of this study, possibly due to the fact that stretch correction was necessary to obtain the laminar burning velocities. A recently constructed chemical kinetic mechanism for diethyl ether oxidation and pyrolysis [20] was compared to experimental results and excellent agreement was achieved. It was found that the flame burning velocities reported in this study compared well to the simulated results. Sensitivity analyses were performed and small species, such as methyl, ethyl and carbon monoxide, were reported to have the greatest effect on the laminar burning velocities of diethyl ether.

Acknowledgements

We would like to acknowledge the support of Science Foundation Ireland under grant number [08/IN1./I2055], the Region Lorraine, the European Commission through the “Clean ICE” Advanced Research Grant of the European Research Council and COST ActionCM0901 towards this work. Support from Judith Würmel in technical writing and Hervé Le Gall in technical assistance during experiments is also greatly appreciated.

References

- [1] K. Kohse-Hoinghaus, P. Osswald, T.A. Cool, T. Kasper, N. Hansen, F. Qi et al., Biofuel combustion chemistry: from ethanol to biodiesel, *Angewandte Chemie International Edition*, 49 (21) (2010), pp. 3572–3597
- [2] D. Pimentel, Ethanol fuels: energy balance, economics, and environmental impacts are negative, *Natural Resources Research*, 12 (2) (2003), pp. 127–134
- [3] B. Bailey, J. Eberhardt, S. Goguen, J. Erwin, Diethyl ether (DEE) as a renewable fuel, *SAE Paper* (1997) 972978

- [4] J.G. Davoud, C.N. Hinshelwood, The thermal decomposition of diethyl ether. Proceedings of the royal society of London series A, Mathematical and Physical Sciences, 171 (944) (1939), pp. 39–54
- [5] G.R. Freeman, C.J. Danby, C. Hinshelwood, The thermal decomposition of diethyl ether. I. Rate-pressure relations. Proceedings of the royal society of London series A, Mathematical and Physical Sciences, 245 (1240) (1958), pp. 28–39
- [6] C.J. Danby, G.R. Freeman, The thermal decomposition of diethyl ether. II. Analytical survey of the reaction products as a function of reaction conditions. Proceedings of the royal society of London series A, Mathematical and Physical Sciences, 245 (1240) (1958), pp. 40–48
- [7] G.R. Freeman, The thermal decomposition of diethyl ether. III. The action of inhibitors and the mechanism of the reaction. Proceedings of the royal society of London series A, Mathematical and Physical Sciences, 245 (1240) (1958), pp. 49–67
- [8] G.R. Freeman, C.J. Danby, The thermal decomposition of diethyl ether. IV. Production of cyanides and the mechanism of the nitric-oxide-induced reaction. Proceedings of the royal society of London series A, Mathematical and Physical Sciences, 245 (1240) (1958), pp. 68–74
- [9] G.R. Freeman, The thermal decomposition of diethyl ether. V. The production of ethanol from diethyl ether and the pyrolysis of ethanol. Proceedings of the royal society of London series A, Mathematical and Physical Sciences, 245 (1240) (1958), pp. 75–83
- [10] D.J. Waddington, The gaseous oxidation of diethyl ether. Proceedings of the royal society of London series A, Mathematical and Physical Sciences, 252 (1269) (1959), pp. 260–272
- [11] K.J. Laidler, D.J. McKenney, Kinetics and mechanisms of the pyrolysis of diethyl ether. I. The uninhibited reaction. Proceedings of the royal society of London series A, Mathematical and Physical Sciences, 278 (1375) (1964), pp. 505–516
- [12] K.J. Laidler, D.J. McKenney, Kinetics and mechanisms of the pyrolysis of diethyl ether. II. The reaction inhibited by nitric oxide. Proceedings of the royal society of London series A, Mathematical and Physical Sciences, 278 (1375) (1964), pp. 517–526
- [13] J.H. Mack, D.L. Flowers, B.A. Buchholz, R.W. Dibble, Investigation of HCCI combustion of diethyl ether and ethanol mixtures using carbon 14 tracing and numerical simulations, Proceedings of Combustion Institute, 30 (2005), pp. 2693–2700
- [14] S. Mosbach, M. Kraft, A. Bhave, F. Mauss, J.H. Mack, R.W. Dibble, Simulating a homogeneous charge compression ignition engine fuelled with a DEE/EtOH blend, SAE Paper (2006) 2006-01-1362
- [15] N.K. Miller Jothi, G. Nagarajan, S. Renganarayanan, Experimental studies on homogeneous charge CI engine fuelled with LPG using DEE as an ignition enhancer, Renewable Energy, 32 (9) (2007), pp. 1581–1593

- [16] K. Sudheesh, J.M. Mallikarjuna, Diethyl ether as an ignition improver for biogas homogenous charge compression ignition (HCCI) operation – an experimental investigation, *Energy*, 35 (9) (2010), pp. 3614–3622
- [17] C. Cinar, O. Can, F. Sahin, Y.H. Serdar, Effects of premixed diethyl ether (DEE) on combustion and exhaust emissions in a HCCI-DI diesel engine, *Applied Thermal Engineering*, 30 (4) (2010), pp. 360–365
- [18] M. Iranmanesh, J.P. Subrahmanyam, M.K.G. Babu, Potential of diethyl ether as a supplementary fuel to improve combustion and emission characteristics of diesel engines, *SAE Paper* (2008) 2008-28-0044
- [19] M. Iranmanesh, J.P. Subrahmanyam, M.K.G. Babu, Potential of diethyl ether as a blended supplementary oxygenated fuel with biodiesel to improve combustion and emission characteristics of diesel engines, *SAE Paper* (2008) 2008-01-1805
- [20] K. Yasunaga, F. Gillespie, J.M. Simmie, H.J. Curran, Y. Kuraguchi, H. Hoshikawa et al., A multiple shock tube and chemical kinetic modeling study of diethyl ether pyrolysis and oxidation, *The Journal of Physical Chemistry A*, 114 (34) (2010), pp. 9098–9109
- [21] W. Agnew, J. Agnew, Visible emission spectra of two-stage flames of diethyl ether produced in flat-flame burner, *Journal of Industrial and Engineering Chemistry*, 48 (12) (1956), pp. 2224–2231
- [22] J.F. Griffiths, T. Inomata, Oscillatory cool flames in the combustion of diethyl ether, *Journal of the Chemical Society, Faraday Transactions*, 88 (21) (1992), pp. 3153–3158
- [23] G.J. Gibbs, H.F. Calcote, Effect of molecular structure on burning velocity, *Journal of Chemical and Engineering Data*, 4 (3) (1959), pp. 226–237
- [24] Y.G. Di, Z.H. Huang, N. Zhang, B. Zheng, X.S. Wu, Z.Y. Zhang, Measurement of laminar burning velocities and Markstein lengths for diethyl ether-air mixtures at different initial pressure and temperature, *Energy and Fuels*, 23 (2009), pp. 2490–2497
- [25] N. Zhang, Y. Di, Z. Huang, B. Zheng, Z. Zhang, Experimental study on combustion characteristics of N₂-diluted diethyl ether-air mixtures, *Energy and Fuels*, 23 (12) (2009), pp. 5798–5805
- [26] N. Zhang, Y.G. Di, Z.H. Huang, Z.Y. Zhang, Flame instability analysis of diethyl ether-air premixed mixtures at elevated pressures, *Chinese Science Bulletin*, 55 (3) (2010), pp. 314–320
- [27] L.P.H. de Goey, A. van Maaren, R.M. Quax, Stabilization of adiabatic premixed laminar flames on a flat flame burner, *Combustion Science and Technology*, 92 (1) (1993), pp. 201–207
- [28] P. Dirrenberger, H. Le Gall, R. Bounaceur, O. Herbinet, P.A. Glaude, A.A. Konnov et al., Measurements of laminar flame velocity for components of natural gas, *Energy and Fuels*, 25 (9) (2011), pp. 3875–3884
- [29] S.G. Davis, C.K. Law, Determination of and fuel structure effects on laminar flame speeds of C₁ to C₈ hydrocarbons, *Combustion Science and Technology*, 140 (1) (1998), pp. 427–449

- [30] K. Saeed, C.R. Stone, Measurements of the laminar burning velocity for mixtures of methanol and air from a constant-volume vessel using a multizone model, *Combustion and Flame*, 139 (1–2) (2004), pp. 152–166
- [31] M. Ó Conaire, H.J. Curran, J.M. Simmie, W.J. Pitz, C.K. Westbrook, A comprehensive modeling study of hydrogen oxidation, *International Journal of Chemical Kinetics*, 36 (2004), pp. 603–622
- [32] D. Healy, D.M. Kalitan, C.J. Aul, E.L. Petersen, G. Bourque, H.J. Curran, Oxidation of C₁-C₅ alkane quinary natural gas mixtures at high pressures, *Energy and Fuels*, 24 (2010), pp. 1521–1528
- [33] W. Lowry, J. de Vries, M. Krejci, E.L. Petersen, Z. Serinyel, W.K. Metcalfe et al., Laminar flame speed measurements and modeling of pure alkanes and alkane blends at elevated pressures, *ASME Conference Proceedings*, 43970 (2010), pp. 855–873
- [34] A. Kéromnès, W.K. Metcalfe, N. Donohoe, H.J. Curran, W.J. Pitz, 7th US national meeting of the combustion institute, Georgia Institute of Technology, Atlanta (2011)
- [35] Metcalfe WK, Burke SM, Aul CJ, Petersen EL, Curran HJ. Proceedings of the European Combustion Meeting, Cardiff, 2011.
- [36] CHEMKIN-PRO 15101, Reaction design, (2010) [San Diego]