

An Investigation on Fuel Similarity of Turbulent Flames for C₄-C₈ *n*-Alkanes

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In this study we experimentally investigated the propagation speed of constant-pressure expanding flames in near-isotropic turbulence using a dual-chamber, fan-stirred vessel. The motivation of the work is to test whether the concept of fuel similarity for C₄-C₈ *n*-alkanes on laminar flames also holds for turbulent flames. Previously it was found that the laminar flame speed, laminar flame thickness and Markstein length are almost identical for these fuels. If this fuel similarity concept can also be shown for turbulent flames, it will suggest a canonical flame structure for large hydrocarbon fuels of the same chemical family, *i.e.*, large fuels always decompose to small C₀-C₄ fuel fragments before being oxidized, and would significantly simplify/generalize the description of such flames. Our preliminary results show that in the flamelet and thin-reaction zone, the turbulent flame speeds of these fuels indeed assume similar values at various pressures, equivalence ratios and turbulence intensities, thereby extending the concept of their fuel similarity to turbulent flame propagation, within the present parametric range of investigation.

1. Introduction

Combustion chemistry of large practical fuels involves thousands of compounds and a large number of reactions, which are difficult to track at a fundamental level. A simplified approach is based on the assumption that large fuels crack rapidly as compared to the subsequent oxidation of cracked intermediates [1,2]. As a result, large fuels do not enter the active oxidation zone directly and it is the oxidation of the cracked products that determines the rates of radical pool build-up and heat release. Hence, a detailed description of the cracking process may not be necessary as long as the major cracked product distribution is well predicted. While such a concept has been proven successful in predicting the global parameters of laminar flames [3–5], its adequacy to model turbulent flames needs to be explored.

Straight-chain species are important components in all practical transportation fuels [6–9] and a number of experimental and modeling efforts have focused on *n*-alkanes [2–4,10–14]. It has been shown that for large *n*-alkanes the laminar flame speeds [3,4,12], flame speed sensitivity to stretch (Markstein lengths) [4], laminar premixed flame extinction strain rates [3] and autoignition delays [10,11,13,14] are largely similar. This supports the use of similarity rules for rates of fuel-related reactions [13]. However, at the same time studies have shown that the ignition and extinction states of non-premixed laminar flames do depend on the carbon chain length [15–17], with the reason attributed to the difference in their diffusivities. Therefore it is of interest to investigate the fuel similarity concept for large *n*-alkanes in more practical systems, such as turbulent flames. Since the coupling between transport and chemistry varies with the turbulence intensity, the extent of fuel similarity is expected to be different at different flow conditions.

In addition, while there are a large number of measurements on laminar flame speeds of large n -alkanes, well-defined measurements on turbulent flame speeds are scarce. Understanding of turbulent flame speeds of n -alkanes can facilitate the prediction and design of practical combustion systems. It is also a useful candidate to validate the performance of kinetic models in turbulent flames, as well as in the development and validation of turbulent combustion models, such as Large Eddy Simulations (LES).

In the present study, turbulent flame speeds for C_5 - C_8 n -alkanes measured using turbulent expanding flames for a wide range of turbulence intensities and equivalence ratios in the pressure range from 1 atm to 5 atm. The results allow direct and consistent assessment of fuel similarity of turbulent flame speeds among n -alkanes under different flow and flame conditions.

2. Experimental Setup

The experiments were conducted in a dual-chamber, fan-stirred, nearly constant-pressure vessel. It has been used for measuring both laminar flame speeds [4,5,18] and turbulent flame speeds [19,20]; detailed description of the experimentation and data analysis are given in the cited references. The vessel incorporates a dual-chamber pressure release technique to allow flame propagation in near constant pressure. The operating conditions are identical to those reported in [19,20], except that now the vessel is heated up to 353 K for experimentation with liquid fuels. The heating is achieved by covering the outer chamber with silicon electrical heaters, hence enabling it to act as an oven to uniformly heat the inner chamber. Turbulence is generated by four orthogonally positioned fans which continuously run during the entire flame propagation event. The fan-generated, non-reacting turbulent flow field was characterized by high-speed particle image velocimetry (HS-PIV). Detailed flow-field statistics and quantification of the small but unavoidable deviation from isotropy are given in [19]. As suggested in [21–23], high-speed Schlieren imaging is particularly suitable for flame speed measurement because of its advantages over other methods, such as laser sheet Mie scattering measurement.

The present study reports data for three fuels: n -pentane, n -hexane and n -octane. The experiments in [4] show that these fuels have almost identical laminar flame speeds, laminar flame thickness and Markstein lengths. Figure 1 plots the conditions of present experiments for n -hexane in the Regime Diagram proposed in [24]. The plots for n -pentane and n -octane are almost the same since all these fuels have similar laminar flame speeds and flame thicknesses. It is seen that most of experiments fall in the corrugate flamelet and thickened flamelet regimes.

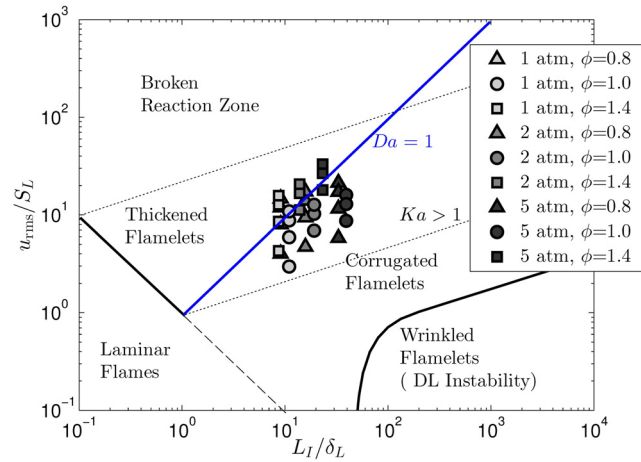


Figure 1: Regime Diagram with conditions of present experiments for n -hexane

3. Results at $\phi = 1.0$ and 1.4

From the Schlieren images, the area A enclosed by the flame edge can be calculated. The mean flame radius is defined as $\langle R \rangle = \sqrt{A/\pi}$. By differentiating the $\langle R \rangle$ history with respect to time, the flame propagation speed $d\langle R \rangle/dt$ can be obtained. The simultaneous measurements using Schlieren imaging and Mie scattering in [23] suggest that $d\langle R \rangle/dt$ corresponds to the turbulent displacement speed corresponding to the progress variable $c = 0.05 \sim 1$. In the following, we will present the data of $d\langle R \rangle/dt$ for different fuels at different conditions.

Throughout the experimental process, we observed a strong dependence on the equivalence ratio from both the Schlieren images and $d\langle R \rangle/dt$ data. For this reason, we will present the data for $\phi = 1.0$ and $\phi = 1.4$ first, which appear to show a different trend for the data for $\phi = 0.8$, to be reported later. In addition, the measurements in [19,20] show that for expanding flames the turbulent flame speed normalized by the laminar flame speed scales well with the square root of a Reynolds number $Re_{T,f}$, defined based on flame radius and flame thickness, i.e.,

$$\frac{1}{S_L} \frac{d\langle R \rangle}{dt} \propto Re_{T,f}^{1/2} = \left(\frac{u_{rms} \langle R \rangle}{S_L \delta_L} \right)^{1/2} \quad (1)$$

Equation (1) was shown to hold for a single combustible mixture (with fixed Lewis number and Markstein number) at different turbulence intensity and pressure. While the present study does not rule out other possibility for scaling of turbulent flame speeds, the fuel similarity in flame speeds will be considered based on Equation (1).

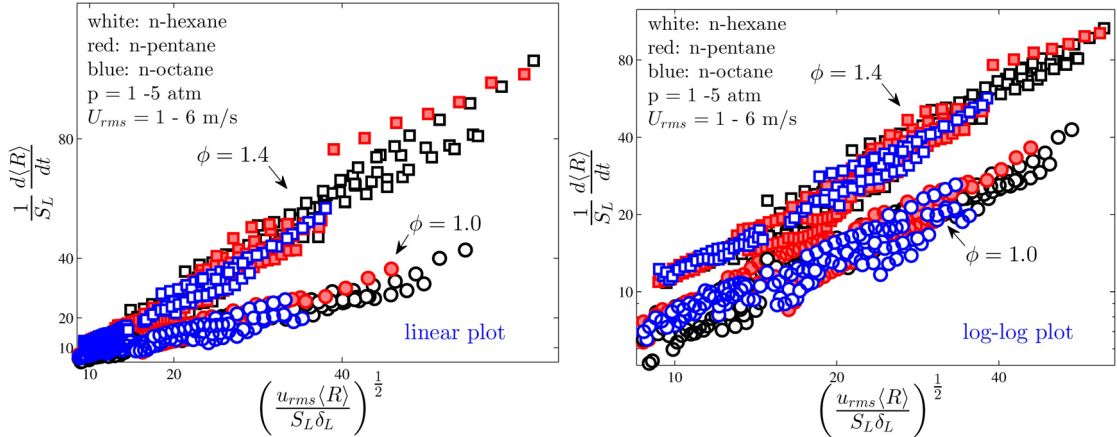


Figure 2: Linear and log-log plots of normalized $d\langle R \rangle/dt$ versus $Re_{T,f}^{0.5}$ for n -pentane, n -hexane and n -octane mixtures with air at $\phi = 1.0$ and $\phi = 1.4$

Figures 2 plots the normalized turbulent flame speeds versus $Re_{T,f}^{1/2}$ at $\phi = 1.0$ and $\phi = 1.4$ for n -pentane, n -hexane and n -octane, respectively. To eliminate the influence of ignition and chamber wall effects, only data in the range $1.0\text{cm} < \langle R \rangle < 2.0\text{cm}$ are considered and plotted. For n -pentane and n -hexane, we were able to obtain data from 1 atm to 5 atm; however, for n -octane data at 5 atm is not possible due to fuel condensation. It is seen that indeed for each individual mixtures, Equation (1) can approximately collapse data obtained at different turbulence intensities, flame radii and pressures. However, the slope of this correlation varies significantly for different mixtures. There is a strong dependence of this slope on the equivalence ratio. Indeed, it is seen that for all three fuels, the normalized turbulent flame speed at $\phi = 1.4$ are much higher than the data at $\phi = 0.8$ for the same $Re_{T,f}$. In [20], this strong variation of slope was explained to be the Markstein diffusion effects, and efforts were made to collapse all the data for C_0 - C_4 and DME by replacing the flame thickness in Equation (1) with the Markstein

lengths. Measurements in [4] reported negative Markstein lengths for $\phi = 1.4$; therefore here we extended the universality of Equation (1) to mixtures with negative Markstein lengths. However, the scaling based on Markstein lengths demonstrated in [20] needs to be extended to cover the data with negative Markstein lengths. In addition, from both the linear plot and log-log plot, it is seen that the data for different fuels collapse reasonable well onto one curve for data at both small and large $Re_{T,f}$. Hence, the validity of fuel similarity for C₅-C₈ n-alkanes is strongly suggested in such conditions.

4. Results at $\phi = 0.8$

We have seen fuel similarity of turbulent flame speeds for stoichiometric and rich mixtures of large *n*-alkanes. So what about fuel lean conditions? We have conducted experiments at $\phi = 0.8$ for various turbulence intensities and pressures. First, we examine the difference between fuel-lean flames and stoichiometric and fuel-rich flames on the flame morphology. Figure 3 shows typical flame images of *n*-octane flames at lean, stoichiometric and rich conditions. It is seen the flame for $\phi = 0.8$ appears quite different from the other two flames. While flame images at $\phi = 1.0$ and $\phi = 1.4$ show clear position of flamefront and sharp flame edge, the flame image at $\phi = 0.8$ shows the opposite. In that the flamefront position is difficult to identify and the burning seems to be spread out into multiple regions.

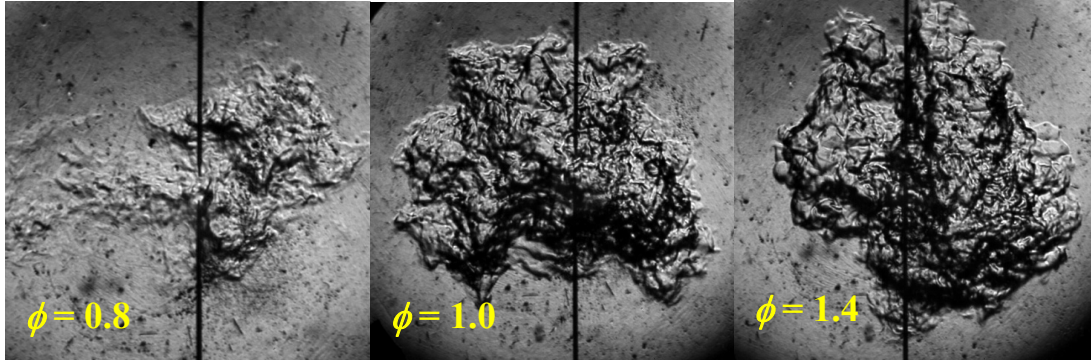


Figure 3: Schlieren images of *n*-octane/air flames at 1 atm with $u_{rms} = 5.24\text{m/s}$ and $rpm = 7500$, $u_{rms} = 5.23\text{m/s}$.

For flames at $\phi = 0.8$, we also clearly observed local extinction as the flame propagates, as shown in Figure 4. The occurrence of local extinction (as versus global extinction) over such a large area also suggests possible re-ignition since extinction leads to unburned hot fuel/air pockets, which might ignite at another instant and location. Thus in spite of the fact that the conditions for $\phi = 0.8$ fall at almost the same location as those for $\phi = 1.0$ and $\phi = 1.4$ in the Regime Diagram, the nature of burning turns out to be quite distinct for these two cases. This then clearly implies that effects of Lewis number need to be incorporated in a more generalized construction of the Regime Diagram.

Local extinction and the blurry flame edge pose significant challenge in tracking or even defining the flame location. In such conditions, technique other than Schlieren imaging may be a better way to identify the flame location, such as HS-PLIF. Nevertheless, we still conducted the tracking using the canny edge detection algorithm in Matlab, which can yield results with reasonably good consistency. In addition, multiple runs were conducted at the same condition to

obtain more averaging. Figure 5 plots normalized turbulent flame speeds versus $Re_{T,f}^{1/2}$ at $\phi = 0.8$ for *n*-pentane, *n*-hexane and *n*-octane. First, it is seen that the data are more scattered than those for $\phi = 1.0$ and $\phi = 1.4$; therefore it is difficult to extract a clear trend from them. Nevertheless, it is still seen that on average the turbulent flame speeds for *n*-octane are lower than *n*-hexane, which in turn are lower than *n*-pentane. The trends seem to suggest that turbulent flame speeds decreases with molecular size. However, more experiments and analysis need to be performed to assure this trend. From Schlieren images, we also found that local extinction for *n*-octane occurs in larger regions than *n*-hexane and *n*-pentane.

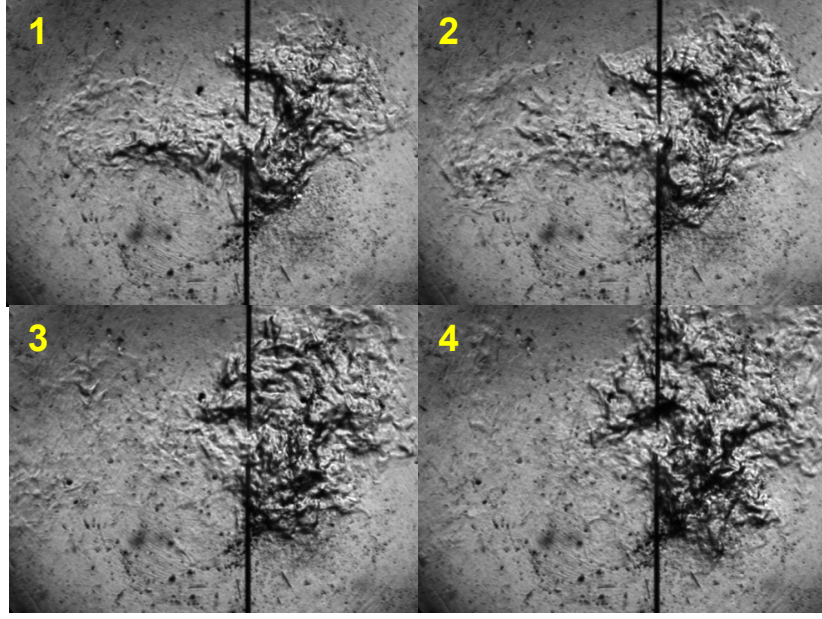


Figure 4: A series of Schlieren images showing large region of local extinction of *n*-octane/air flame at $\phi = 0.8$, 1 atm with $u_{rms} = 5.24\text{m/s}$ and $rpm = 7500$, $u_{rms} = 5.23\text{m/s}$. The numbers indicate the sequence of flame propagation.

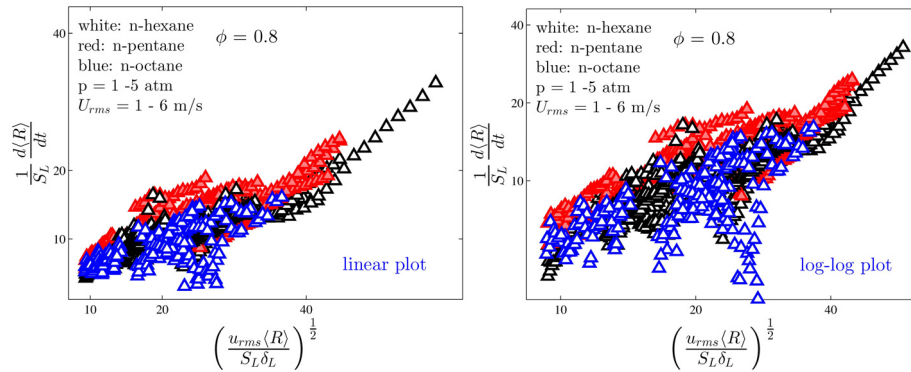


Figure 5: Linear and log-log plots of normalized $d\langle R \rangle / dt$ versus $Re_{T,f}^{0.5}$ for *n*-pentane, *n*-hexane and *n*-octane mixtures with air at $\phi = 0.8$

5. Concluding Remarks

The present study measured the turbulent flame speeds for *n*-pentane, *n*-hexane and *n*-octane for a wide range of parameters from 1 atm to 5 atm using expanding turbulent flames in a fan-stirred vessel. The primary motivation is to verify fuel similarity of turbulent flame speeds for large *n*-alkanes. Results show that for stoichiometric and rich mixtures (near-unity *Le*, or *Le* < 1), the turbulent flame speeds of C₅-C₈ *n*-alkanes are almost the same. However, for lean mixtures (*Le* > 1) of all fuels, large regions of local extinction are observed from the Schlieren images and data of turbulent flame speeds have large scattering. Upon averaging, the data suggested that at lean conditions, the turbulent flame speeds decrease with the carbon number of the fuel.

Acknowledgments

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References

- [1] X. You, F.N. Egolfopoulos, H. Wang, Proceedings of the Combustion Institute 32 (2009) 403.
- [2] H. Wang, E. Dames, B. Sirjean, D.A. Sheen, R. Tangko, A. Violi, J.Y.W. Lai, F.N. Egolfopoulos, D.F. Davidson, R.K. Hanson, C.T. Bowman, C.K. Law, N.P. Cernansky, D.L. Miller, R.P. Lindstedt, University of Southern California (2010).
- [3] C. Ji, E. Dames, Y.L. Wang, H. Wang, F.N. Egolfopoulos, Combustion and Flame 157 (2010) 277.
- [4] A.P. Kelley, A.J. Smallbone, D.L. Zhu, C.K. Law, Proceedings of the Combustion Institute 33 (2011) 963.
- [5] F. Wu, A.P. Kelley, C.K. Law, Combustion and Flame 159 (2012) 1417.
- [6] A. Violi, S. Yan, E.G. Eddings, A.F. Sarofim, S. Granata, T. Faravelli, E. Ranzi, Combustion Science and Technology 174 (2002) 339.
- [7] W.J. Pitz, N.P. Cernansky, F.L. Dryer, F.N. Egolfopoulos, J.T. Farrell, D.G. Friend, in: Society of Automotive Engineers, 2007, pp. 2007-01-0175.
- [8] J.T. Farrell, N.P. Cernansky, F.L. Dryer, D.G. Friend, C.A. Hergart, C.K. Law, R.M. McDavid, C.J. Mueller, A.K. Patel, H. Pitsch, in: Society of Automotive Engineers, 2007, pp. Paper 2007-01-0201.
- [9] M. Colket, T. Edwards, S. Williams, N.P. Cernansky, D.L. Miller, F.N. Egolfopoulos, P. Lindstedt, K. Seshadri, F.L. Dryer, C.K. Law, D. Friend, D.B. Lenhert, H. Pitsch, A. Sarofim, M. Smooke, W. Tsang, in: American Institute of Aeronautics and Astronautics, 2007, p. Paper 2007-770.
- [10] D.F. Davidson, S.C. Ranganath, K.-Y. Lam, M. Liaw, Z. Hong, R.K. H., Journal of Propulsion and Power 26 (2010) 280.
- [11] H.S. Shen, J. Steinberg, J. Vanderover, M.A. Oehlschlaeger, R. V December, V. Re, M. Recei, V. February, Energy & Fuels 23 (2009) 2482.
- [12] S.G. Davis, C.K. Law, Combustion Science and Technology 140 (1998) 427.
- [13] C.K. Westbrook, W.J. Pitz, O. Herbinet, H.J. Curran, E.J. Silke, Combustion and Flame 156 (2009) 181.
- [14] E. Ranzi, A. Frassoldati, S. Granata, T. Faravelli, Industrial and Engineering Chemistry Research 44 (2005) 5170.
- [15] W. Liu, J.A. Koch, C.K. Law, Combustion and Flame (2011).
- [16] S.H. Won, S. Dooley, F.L. Dryer, Y. Ju, Combustion and Flame 159 (2012) 541.
- [17] A.T. Holley, X.Q. You, E. Dames, H. Wang, F. . Egolfopoulos, Proceedings of the Combustion Institute 32 (2009) 1157.
- [18] F. Wu, C.K. Law, Combustion and Flame in Press (2013).
- [19] S. Chaudhuri, F. Wu, D. Zhu, C.K. Law, Physical Review Letters 108 (2012) 044503.
- [20] S. Chaudhuri, F. Wu, C.K. Law, Physical Review E 003000 (2013).
- [21] D. Bradley, M.Z. Haq, R. a. Hicks, T. Kitagawa, M. Lawes, C.G.W. Sheppard, R. Woolley, Combustion and Flame 133 (2003) 415.
- [22] M. Lawes, M.P. Ormsby, C.G.W. Sheppard, R. Woolley, Combustion and Flame 159 (2012) 1949.
- [23] D. Bradley, M. Lawes, M.S. Mansour, Combustion and Flame 158 (2011) 123.
- [24] N. Peters, Journal of Fluid Mechanics 384 (1999) 107.