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Inferences about the mechanism of flame stabilization in the near-field of diesel jets

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Abstract

Several mechanisms to explain flame stabilization at the lift-off height in a turbulent jet have been proposed in the literature. These include strain-induced extinction of a propagating flame, balance of flow and flame velocities, and re-entrainment of product gases. More recently, experiments have suggested that there may be a correlation between ignition characteristics and flame lift-off. In this work, simulations of ignition, ignition front propagation, flame propagation, and flame stabilization employing an unsteady flamelet progress variable model in turbulent reacting diesel jets reveal that the flame stabilization point coincides with the ignition strain rate in the jet. Comparisons of computed and measured flame lift-off heights are presented over a wide range of injection velocity, ambient temperature and density, and ambient oxygen concentration conditions. The results are critically examined to provide insight into the mechanism of flame stabilization in a diesel jet.

Introduction

Predicting the lift-off heights accurately in diesel jets is important, because it has been shown that changes in lift-off height which reflects changes in fuel/air mixing upstream of the lift-off height influences soot formation in the jet. Flame lift-off in jets has been a subject of extensive research and discussion for the past four decades [7,9]. Several theories have been proposed based on experimental and numerical investigations. Some of the important ideas will be briefly discussed. It has been proposed that the diffusion flame on a burner will lift when the mean velocity gradient at the burner exceeds a certain critical value, and that it will stabilize at the position where the burning velocity is equal to mean flow velocity, i.e. $U_s = S_T$ in Fig. 1 [23,25,26]. Measurements of concentration fluctuations in turbulent propane jets [18] have, however, shown that the assumption of complete premixing at the flame base may not be appropriate.

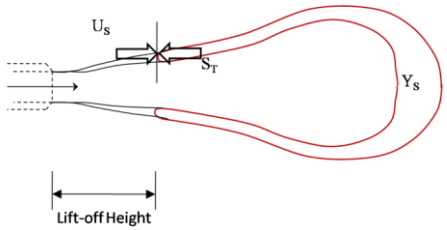

Figure 1. Illustration of theory of premixedness [24].

Peters and Williams [15] argued that there is insufficient time below the base of the flame to achieve the degree of premixedness required to support the concept of premixed combustion. Therefore, they suggested that the lift-off height occurs where the flame is extinguished by large strain rates, i.e. lift-off would occur at the location where the local stoichiometric scalar dissipation rate χ_{st} exceeds the extinction limit χ_q for a laminar diffusion flamelet. Venugopal and Abraham [24] employed this theory to model flame lift-off in diesel jets. For the range of conditions considered, they showed that the results were consistent with experimental results [20,21]. Broadwell *et al.* [3] postulated that large scale eddies are responsible for carrying the hot combustion products from a downstream location into the jet upstream. These entrained products helps to ignite the non-combusting eddies of the jet. According to this model, the lift-off height is achieved when the mixing rate of the re-entrained products is such that there is insufficient time for the reactions to occur before the temperature of the hot gases decreases, i.e. the lift-off height is dependent on the interplay between the chemical and mixing times. Müller *et al.* [13] proposed that both premixed flame propagation and diffusion flame extinction effects are important in flame stabilization. They and others [14] have suggested a triple flame propagating along the mixing layer after ignition, and extinction of the triple flame at the lift-off height.

This discussion shows that, many years of research notwithstanding, the understanding of flame stabilization is not complete. In fact, in diesel jets models based on different proposals explaining the lift-off process have been employed to predict the same lift-off data. These includes models based on partially stirred reactor (PaSR) theory in combination with multi-step chemical kinetics [10], perfectly stirred reactor (PSR) theory with multi-step kinetics [11], flame surface density evolution [13], diffusion flamelet extinction [24,25], and a combination of eddy-dissipation and PSR time scales [5].

In recent work, the authors have shown that an unsteady flamelet progress variable (UFPV) model can reproduce the ignition delay and flame lift-off in diesel jets over a wide range of conditions within approximately 25%. This paper examines what this success informs us about the mechanism of flame stabilization. In other words, why does the model predict the results with reasonable accuracy? The model will be briefly discussed below. Some results will then be presented. The critical discussion will then follow and the paper will end with conclusions.

The Computational Model

In the UFPV model [6,17], the chemical source terms are obtained by solving the equations for the unsteady flamelet and tabulating the reaction rates in look-up tables as a function of three independent parameters: the mixture fraction Z, and the progress variable C_{st} and the scalar dissipation rate estimated at the stoichiometric mixture fraction, χ_{st}. In general, C is a function of Z. To simplify the look-up table, the assumption is

made that the C(Z) profile can be characterized by the stoichiometric value of C, i.e. C_{st}. This profile is obtained from a separate look-up table where C(Z) is tabulated for different values of C_{st} during the transient evolution of the flamelet. There is an implicit assumption that given a value of C_{st}, the C at any Z is unique. Refs. [11, 12] has shown that this is a reasonable assumption. This is analogous to the treatment of χ(Z) in combustion models [12]. Note that C(Z) values can be obtained for both igniting and extinguishing flames. In RANS simulations, the average source terms are required. These can be obtaining by convolving the instantaneous source terms in the look-up table with the joint probability density function (PDF), $\tilde{P}(Z, C_{st}, \chi_{st})$, of the independent variables, i.e.

$$\tilde{\omega}_{\varphi} = \iiint \dot{\varphi} \tilde{P}(Z, C_{st}, \chi_{st})\, dZ dC_{st} d\chi_{st}, \quad (1)$$

where ~ denotes Fávre averaging. In the UFPV implementation reported in the literature, the assumption is made that the PDFs of the independent variables are statistically independent of each other. This assumption has also been assessed in detail in Refs. [11,12]. Statistical independence converts the conditional PDFs into their respective marginal PDFs, i.e.

$$\tilde{P}(Z, C_{st}, \chi_{st}) = \tilde{P}(Z)\tilde{P}(C_{st})\tilde{P}(\chi_{st}). \quad (2)$$

Presumed functional forms will be employed to approximate the shapes of the PDFs of the three variables Z, C_{st} and χ_{st}. The β-PDF is employed for Z and (for simplicity) δ-PDFs for C_{st} and χ_{st}. These assumptions are evaluated in detail in Refs. [11,12].

Results and Discussions

The measured values of ignition delay and lift-off height were obtained in a constant-volume chamber and they are available on the Engine Combustion Network maintained by Sandia National Laboratories, Livermore, CA (http://www.ca.sandia.gov/ECN). n-Heptane was employed as the fuel. A skeletal mechanism for n-heptane oxidation consisting of 44-species and 185 reactions is employed to represent the kinetics [8]. A RANS code that has been employed in prior work for computing similar sprays (and vapor jets) was employed in this work. Refs. [1, 2, 19] discuss the models employed and the justification for using sprays and/or vapor jets to represent the fuel jets. Table 1 lists nine cases simulated in this work. The variables d_{noz}, d_{gas}, P_{inj}, P_{amb}, T_{amb}, ρ_{amb}, and O_2% represent the nominal orifice diameter, the equivalent orifice diameter when the fuel is injected as vapor [1], the injection pressure, the chamber pressure, the chamber temperature, the chamber density, and the oxygen percentage in the chamber on a mole basis.

Case	d_{noz} mm	d_{gas} mm	P_{inj} MPa	P_{amb} bar	T_{amb} K	ρ_{amb} kg/m^3	O_2%
1	0.1	0.199	150	42.66	1000	14.8	21
2	0.1	0.199	60	42.66	1000	14.8	21
3	0.1	0.1745	150	55.45	1300	14.8	21
4	0.1	0.2907	150	38.39	900	14.8	21
5	0.1	0.199	150	43.02	1000	14.8	15
6	0.1	0.199	150	43.2	1000	14.8	12
7	0.1	0.199	150	43.45	1000	14.8	8
8	0.18	0.3858	140	42.66	1000	14.8	21
9	0.1	0.1397	150	86.47	1000	30.0	15

Table 1. Computational conditions

Figure 2 shows the transient evolution of the temperature contours for Case 1. The jet initially penetrates into the chamber without significant rise in temperature. Higher scalar dissipation rates retard ignition in the near field. The first significant rise in temperature is observed at 0.55 ms ASI. Subsequent to this, a front propagates upstream through the stoichiometric mixture. Beyond about 1.0 ms, the front no longer propagates upstream, i.e. a steady lift-off height is achieved. Table 2 shows the computed and measured ignition delays and lift-off heights for the different cases.

Table 2 can be understood from this perspective. Case 2 has lower injection pressure which results in lower scalar dissipation rates in the near-field of the jet relative to Case 1 thereby enabling the propagating front to travel farther upstream relative to Case 1. Case 3 has a higher chamber temperature increasing the ignition strain rate of the flame whereas the scalar dissipation rates in the near-field of the jet remain the same as in Case 1. The flame can propagate farther upstream before the ignition scalar dissipation rate is matched by the local scalar dissipation rate. The opposite effect is shown for Case 4 where the chamber temperature is lower. Cases 5-7 and 9 can also be explained in this way. In Case 8, the orifice diameter is increased and the lift-off height increases. Note that the injection velocity in Case 8 is the same as in Case 1. With increasing orifice diameter, the fuel injection rate increases. From scaling laws, it can be shown that the ratio of mass of air entrained to mass injected decreases inversely with increasing diameter. When lesser mass is entrained (in a relative sense), the scalar dissipation rate decreases slower with axial distance. Hence, the ignition scalar dissipation rate is equal to the local scalar dissipation rate at a greater axial distance in the jet.

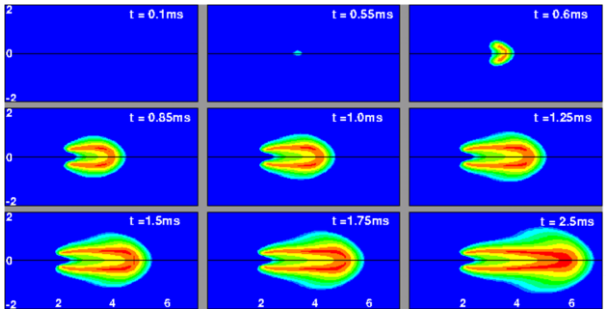

Figure 2: Transient development of temperature contours for Case 1.

Case	Ignition Delay τ_{id} (ms)		Lift-off Height L_F (mm)	
	Measured	Computed	Measured	Computed
1	0.53	0.542	17	18.5
2	-	0.615	13.5[a]	15.05
3	0.26	0.209	7.7	8.05
4	0.79	0.89	25.5	23.3
5	0.73	0.56	23.2	22.9
6	0.947	1.225	29.2	27.3
7	1.52	2.17	42.3	52.88
8	0.57	0.65	23.97	25.8
9	0.38	0.175	11.9	12

Table 2. Computed and measured ignition delay and lift-off height

Figure 3 shows the conceptual picture of the transient evolution of the reacting diesel spray. The liquid length reaches a steady value [4,19,22] a short period after injection. Subsequently, as the vapor fuel penetrates into the chamber, low-temperature and intermediate temperature chemical reactions occur. These reactions lead to autoignition of the mixture. Ignition typically occurs in a richer mixture (Z ~ 0.1-0.2) toward the leading tip of the jet and then an ignition front propagates from the rich mixture to the stoichiometric mixture (Z ~ 0.062) [4]. Once the ignition front reaches the stoichiometric mixture, the flame front propagates along the stoichiometric boundary until the lift-off height is achieved. When the UFPV model is employed, the propagation of the flame is achieved by heat diffusion to and temperature rise in upstream cells. The heat diffusion raises the value of the progress variable *C*. Reaction rates corresponding to the higher value of *C* are fetched from the look-up table which accelerates the rise in temperature and so on. In this way temperature rises in upstream cells.

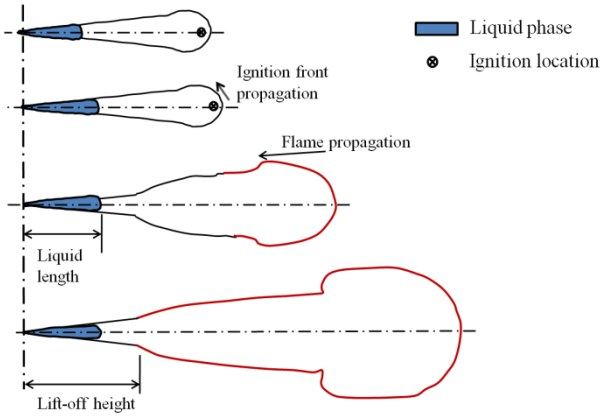

Figure 3. Schematic illustrating the development of a reacting diesel jet

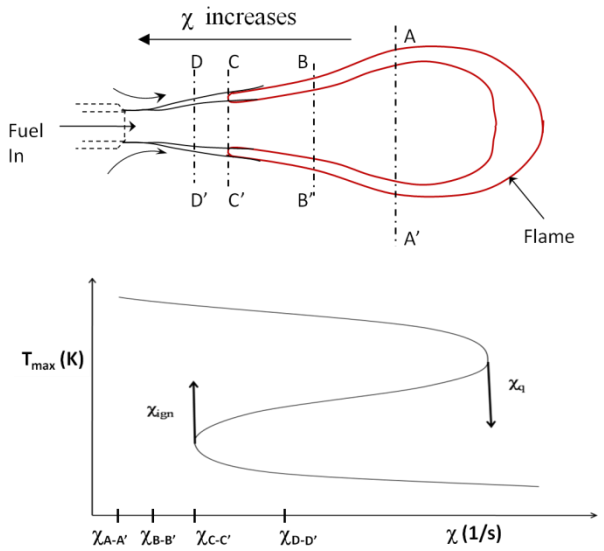

Figure 4. Schematic illustrating variation of scalar dissipation rate in the jet and relation to the S-curve

The process of flame propagation continues as long the scalar dissipation rate χ has a value that lies below the ignition limit. Figure 4 shows the typical S-curve which characterizes ignition and extinction behavior of mixtures. Also shown is the schematic of a jet. Sections A-A` and B-B` lie upstream of the lift-height, and the corresponding scalar dissipation rates are shown on the S-curve. Notice that these scalar dissipation rates are lower than the ignition limiting scalar dissipation rate. As the flame propagates upstream from section A-A` to B-B` the scalar dissipation rate increases. Section C-C` identifies the plane where the flame finally stabilizes. At this section, the scalar dissipation rate corresponds to the ignition limiting scalar dissipation rate χ_{ign}. There is experimental evidence to suggest that the lift-off height in diesel jets is related to the ignition process. Pickett et al. [16] conducted experiments in diesel jets injected into a constant-volume chamber and measured lift-off heights. From their analysis of OH chemiluminescence images, the authors conclude that ignition processes are closely related to lift-off. Their results show that fuels with shorter ignition delays have shorter lift-off height. They observed cool flames just upstream of the quasi-steady lift-off height. The presence of the cool flame suggests that the first-stage of ignition in a two-stage ignition fuel influences lift-off. It is unclear whether lift-off is established through a second-stage ignition of the cool flame or due to upstream flame propagation at high speeds. They also showed from the analysis of the lift-off database of Siebers and Higgins [20] and Siebers et al. [21] that the residence time from the orifice to the lift-off height in the jet fits into an Arrhenius-type expression similar to that employed in the literature for ignition delay. The precise connection between the argument advanced in the current paper and their findings is not clear. It is possible that the ignition scalar dissipation rate that is discussed above can be related to ignition delay or other fuel properties. This requires further study.

Summary and Conclusions

Several mechanisms have been proposed in the literature to explain flame stabilization in turbulent reacting jets. In the case of diesel jets, the same experimental data can be reasonably well predicted by turbulent combustion models which are based on different assumptions about lift-off physics. While this paper does not seek to answer why different mechanisms explain flame lift-off in diesel jets, recent results for diesel jet autoignition and flame lift-off studies are critically examined to provide insight into the possible mechanism of flame lift-off. In other words, what does the ability of the model to predict the lift-off say about the lift-off mechanism? It is shown that the flame is stabilized at the plane where the local scalar dissipation rate is equal to the ignition scalar dissipation rate along the stoichiometric surface. This result is consistent with recent suggestion about the dependence of the lift-off height in diesel jets on ignition characteristics of fuels. The precise linkage between the findings in this paper and the suggestions made by the earlier researchers need to be established through further work.

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